Quicksort Asymptotics

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ABSTRACT

The number of comparisons X_n used by `Quicksort` to sort an array of n distinct numbers has mean μ_n of order $n \log n$ and standard deviation of order n. Using different methods, Régnier and Rösler each showed that the normalized variate $Y_n := (X_n - \mu_n)/n$ converges in distribution, say to Y; the distribution of Y can be characterized as the unique fixed point with zero mean of a certain distributional transformation.

We provide the first rates of convergence for the distribution of Y_n to that of Y, using various metrics. In particular, we establish the bound $2n^{-1/2}$ in the d_2-metric, and the rate $O(n^{\varepsilon-(1/2)})$ for Kolmogorov–Smirnov distance, for any positive ε.

AMS 2000 *subject classifications.* Primary 68W40; secondary 68P10, 60F05, 60E05.

Key words and phrases. `Quicksort`, sorting algorithm, asymptotics, limit distribution, rate of convergence, Kolmogorov–Smirnov distance, density, moment generating function, numerical analysis, d_p-metric, coupling.

Date. May 30, 2002.

[1]Research supported by NSF grants DMS–9803780 and DMS–0104167, and by The Johns Hopkins University's Acheson J. Duncan Fund for the Advancement of Research in Statistics; carried out in part while author was Visiting Researcher, Theory Group, Microsoft Research.

1 Introduction and summary

This paper provides the first rates of convergence (as $n \to \infty$) for the distribution of the number of comparisons used by the sorting algorithm `Quicksort` to sort an array of n distinct numbers. `Quicksort` is the standard sorting procedure in `Unix` systems, and has been cited [3] as one of the ten algorithms "with the greatest influence on the development and practice of science and engineering in the 20th century." We begin with a brief review of what is known about the analysis of `Quicksort` and a summary of our new results.

The `Quicksort` algorithm for sorting an array of n distinct numbers is extremely simple to describe. If $n = 0$ or $n = 1$, there is nothing to do. If $n \geq 2$, pick a number uniformly at random from the given array. Compare the other numbers to it to partition the remaining numbers into two subarrays. Then recursively invoke `Quicksort` on each of the two subarrays.

Let X_n denote the (random) number of comparisons required (so that $X_0 = 0$). Then X_n satisfies the distributional recurrence relation

$$X_n \stackrel{\mathcal{L}}{=} X_{U_n - 1} + X^*_{n-U_n} + n - 1, \qquad n \geq 1, \tag{1.1}$$

where $\stackrel{\mathcal{L}}{=}$ denotes equality in law (i.e., in distribution), and where, on the right, U_n is distributed uniformly on the set $\{1, \ldots, n\}$, $X^*_j \stackrel{\mathcal{L}}{=} X_j$, and

$$U_n;\ X_0, \ldots, X_{n-1};\ X^*_0, \ldots, X^*_{n-1}$$

are all independent.

As is well known and quite easily established, for $n \geq 0$ we have

$$\mu_n := \mathbf{E}\, X_n = 2(n+1)H_n - 4n \sim 2n \ln n,$$

where $H_n := \sum_{k=1}^n k^{-1}$ is the nth harmonic number and $\sim$ denotes asymptotic equivalence. It is also routine to compute explicitly the variance of X_n (see Exercise 6.2.2-8 in [15]):

$$\mathbf{Var}\, X_n = 7n^2 - 4(n+1)^2 H_n^{(2)} - 2(n+1)H_n + 13n = \sigma^2 n^2 - 2n \ln n + O(n) \tag{1.2}$$

where $H_n^{(2)} := \sum_{k=1}^n k^{-2}$ are the second-order harmonic numbers and, using the standard notation $\doteq$ for approximate equality,

$$\sigma^2 := 7 - \tfrac{2}{3}\pi^2 \doteq 0.4203. \tag{1.3}$$

Consider the normalized variate

$$Y_n := (X_n - \mu_n)/n, \qquad n \geq 1.$$

Then (1.1) implies the recursion

$$Y_n \stackrel{\mathcal{L}}{=} \frac{U_n - 1}{n} Y_{U_n - 1} + \frac{n - U_n}{n} Y^*_{n-U_n} + C_n(U_n), \qquad n \geq 1, \tag{1.4}$$

with Y_0 arbitrarily defined (since its coefficient is 0), where on the right, as for X_n, we have $U_n \sim \text{unif}\{1,\dots,n\}$ and $Y_j^* \overset{\mathcal{L}}{=} Y_j$, and $U_n;\ Y_1,\dots,Y_{n-1};\ Y_1^*,\dots,Y_{n-1}^*$ are all independent; further,

$$C_n(i) := \tfrac{n-1}{n} + \tfrac{1}{n}(\mu_{i-1} + \mu_{n-i} - \mu_n), \quad 1 \le i \le n. \tag{1.5}$$

Note that $\mathbf{E}\, Y_n = 0 = \mathbf{E}\, C_n(U_n)$. We will see below that if $n \to \infty$ and $i/n \to u \in [0,1]$, then $C_n(i) \to C(u)$, where

$$C(u) := 2u \ln u + 2(1-u)\ln(1-u) + 1, \qquad u \in [0,1],$$

with the natural (continuous) interpretation $C(u) := 1$ for $u = 0, 1$.

Moreover, Régnier [18] and Rösler [19] showed, using different methods, that $Y_n \to Y$ in distribution, and Rösler also showed that Y satisfies the distributional identity

$$Y \overset{\mathcal{L}}{=} UY + (1-U)Y^* + C(U) \tag{1.6}$$

obtained by formally taking limits in (1.4), where, on the right, U, Y, and Y^* are independent, with $Y^* \overset{\mathcal{L}}{=} Y$ and $U \sim \text{unif}(0,1)$. [Rösler [19] showed further that (1.6) characterizes the limiting law $\mathcal{L}(Y)$, subject to $\mathbf{E}\, Y = 0$ and $\mathbf{Var}\, Y < \infty$. For a complete characterization of the distributions satisfying (1.6), see [7].]

The purpose of the present paper is to study the rate of convergence of $\mathcal{L}(Y_n)$ to $\mathcal{L}(Y)$, using several different measures of the distance between $\mathcal{L}(Y_n)$ and $\mathcal{L}(Y)$.

First, for real $1 \le p < \infty$, let $\|X\|_p := (\mathbf{E}\,|X|^p)^{1/p}$ denote the L^p-norm, and let d_p denote the metric on the space of all probability distributions with finite pth absolute moment defined by

$$d_p(F,G) := \min \|X - Y\|_p,$$

taking the minimum over all pairs of random variables X and Y (defined on the same probability space) with $\mathcal{L}(X) = F$ and $\mathcal{L}(Y) = G$. We will use the fact [1] that the minimum is attained for each $1 \le p < \infty$ by the same X and Y, viz., $X := F^{-1}(u)$ and $Y := G^{-1}(u)$ defined for u in the probability space $(0,1)$ (with Lebesgue measure).

We will for simplicity write $d_p(X,Y) := d_p(\mathcal{L}(X), \mathcal{L}(Y))$ for random variables X and Y, but note that this distance depends only on the marginal distributions of X and Y.

Rösler [19] showed that $d_p(Y_n, Y) \to 0$ as $n \to \infty$ for every $1 \le p < \infty$. In Sections 2 and 3 we will quantify this and show that

$$d_p(Y_n, Y) = O\left(n^{-1/2}\right)$$

for every fixed p. In the case $p = 2$ we will further show the explicit bound

$$d_2(Y_n, Y) < 2n^{-1/2}.$$

The best lower bound we can show (Section 4) is

$$d_p(Y_n, Y) \ge c\frac{\ln n}{n}, \qquad p \ge 2,$$

with $c > 0$ independent of p. We do not know what the correct rate is, even for $p = 2$. In an earlier draft of this paper, we conjectured the rate $n^{-1/2}$. Subsequent to that draft, however, Neininger and Rüschendorf [17] surprisingly showed that for another metric, namely, the Zolotarev metric ζ_3, the correct rate is $(\ln n)/n$. We therefore now guess that the rate is also $(\ln n)/n$ for the metrics d_p, matching our lower bound—but proving this is a challenge.

In Section 5 we use these results to bound the Kolmogorov–Smirnov distance $d_{\mathrm{KS}}(Y_n, Y)$ between $\mathcal{L}(Y_n)$ and $\mathcal{L}(Y)$. We show that

$$d_{\mathrm{KS}}(Y_n, Y) = O\left(n^{\varepsilon-(1/2)}\right)$$

for every $\varepsilon > 0$. Again we do not know the exact rate, but guess that it is $(\ln n)/n$, as for the ζ_3 metric considered by Neininger and Rüschendorf [17]. The best lower bound we can prove is c/n with $c > 0$.

In Section 6 we prove a kind of local limit theorem which enables us to approximate the density function f of Y. (It was proved by Tan and Hadjicostas [20] that Y has a density function; f is bounded and infinitely differentiable by [6].)

Rösler [19] showed that (for fixed $\lambda \in \mathbf{R}$) the moment generating function values $\mathbf{E}\, e^{\lambda Y_n}$ are bounded and thus converge to $\mathbf{E}\, e^{\lambda Y}$. Again we quantify his bounds and give in Section 7 explicit bounds, based on Rösler's method.

In several (but not all) bounds we give explicit numerical values to constants. These values are hardly the best possible, but we make some effort to get fairly small values. This includes sometimes the use of extensive numerical verifications by computer for small n. [All numerical calculations have been verified independently by the two authors, the (alphabetically) first using `Mathematica` and the second using `Maple`.] Such arguments could be simplified or omitted at the cost of increasing the constants.

1.1 Preliminaries

In order to later estimate $C_n(i)$ defined by (1.5) we need some explicit bounds on μ_n. First, as mentioned above,

$$\mu_n = 2(n+1)H_n - 4n, \tag{1.7}$$

which can be rewritten

$$\mu_n = 2(n+1)H_{n+1} - 4n - 2. \tag{1.8}$$

Next we use the bounds on the harmonic numbers (see, e.g., Section 1.2.11.2 in [14])

$$\ln n + \gamma \le H_n \le \ln n + \gamma + \tfrac{1}{2n}, \qquad n \ge 1, \tag{1.9}$$

where $\gamma \doteq 0.5772$ is Euler's constant. Hence, for $n \ge 1$, from (1.7)

$$2(n+1)\ln n + (2\gamma - 4)n + 2\gamma \le \mu_n \le 2(n+1)\ln n + (2\gamma - 4)n + 2\gamma + \tfrac{n+1}{n} \tag{1.10}$$

and from (1.8)

$$2n \ln n + (2\gamma - 4)n + 2 \le \mu_{n-1} \le 2n \ln n + (2\gamma - 4)n + 3. \tag{1.11}$$

2 Bounding $d_2(Y_n, Y)$

In this section we prove the following explicit estimate for $d_2(Y_n, Y)$.

Theorem 2.1. *For all $n \geq 1$, $d_2(Y_n, Y) < 2/\sqrt{n}$.*

Proof. We basically follow the method of Rösler [19], making all estimates explicit. We study in this paper only properties of the univariate distributions of Y_n. We thus take the liberty of letting Y_n denote any random variable with the appropriate distribution $[Y_n \stackrel{\mathcal{L}}{=} (X_n - \mu_n)/n]$. We then may choose $Y_0, Y_1, \ldots$ defined on the same probability space as Y and such that

$$\|Y_n - Y\|_2 = d_2(Y_n, Y), \qquad n \geq 0.$$

Further, let $(Y^*, Y_0^*, Y_1^*, \ldots)$ be an independent copy of $(Y, Y_0, Y_1, \ldots)$ and let $U \sim \text{unif}(0,1)$ be independent of everything else. For convenience we write $a_n := d_2(Y_n, Y)$.

Observe, by (1.4), that

$$Y_n \stackrel{\mathcal{L}}{=} \tilde{Y}_n := \frac{\lceil nU \rceil - 1}{n} Y_{\lceil nU \rceil - 1} + \frac{n - \lceil nU \rceil}{n} Y^*_{n - \lceil nU \rceil} + C_n(\lceil nU \rceil) \tag{2.1}$$

and recall from (1.6) that

$$Y \stackrel{\mathcal{L}}{=} \tilde{Y} := UY + (1-U)Y^* + C(U). \tag{2.2}$$

Therefore,

$$a_n^2 = d_2^2(Y_n, Y) \leq \mathbf{E}\,|\tilde{Y}_n - \tilde{Y}|^2. \tag{2.3}$$

Now

$$\begin{aligned}\tilde{Y}_n - \tilde{Y} &= \left(\frac{\lceil nU \rceil - 1}{n} Y_{\lceil nU \rceil - 1} - UY\right) + \left(\frac{n - \lceil nU \rceil}{n} Y^*_{n - \lceil nU \rceil} - (1-U)Y^*\right) \\ &\qquad + (C_n(\lceil nU \rceil) - C(U)) \\ &=: W_1 + W_2 + W_3,\end{aligned}$$

say. Given U, the random variables W_1 and W_2 are independent with zero mean, while W_3 is a constant. Hence

$$\mathbf{E}\left(\left|\tilde{Y}_n - \tilde{Y}\right|^2 \,\middle|\, U\right) = \mathbf{E}\left((W_1 + W_2 + W_3)^2 \,\middle|\, U\right) = \mathbf{E}\left(W_1^2 \,|\, U\right) + \mathbf{E}\left(W_2^2 \,|\, U\right) + W_3^2$$

and thus, taking expectations,

$$\mathbf{E}\left|\tilde{Y}_n - \tilde{Y}\right|^2 = \mathbf{E}\,W_1^2 + \mathbf{E}\,W_2^2 + \mathbf{E}\,W_3^2. \tag{2.4}$$

By symmetry (replacing U by $1-U$), $\mathbf{E}\,W_2^2 = \mathbf{E}\,W_1^2$. We estimate this term by conditioning on U, using the independence of U and $Y, Y_0, \ldots$. If $U = (k+v)/n$, with

$k \in \{0, 1, \dots, n-1\}$ and $0 < v \le 1$, then $\lceil nU \rceil = k+1$ and $W_1 = \frac{k}{n}(Y_k - Y) - \frac{v}{n}Y$; hence Minkowski's inequality yields

$$\begin{aligned}\mathbf{E}\left(W_1^2 \,|\, U = (k+v)/n\right)^{1/2} &\le \tfrac{k}{n}\|Y_k - Y\|_2 + \tfrac{v}{n}\|Y\|_2 \\ &= \tfrac{k}{n}a_k + \tfrac{v}{n}\sigma.\end{aligned}$$

Consequently,

$$\begin{aligned}\mathbf{E}\,W_1^2 &= \frac{1}{n}\sum_{k=0}^{n-1}\int_0^1 \mathbf{E}\left(W_1^2 \,|\, U = (k+v)/n\right)\,dv \le \frac{1}{n}\sum_{k=0}^{n-1}\int_0^1\left(\frac{k}{n}a_k + \frac{v}{n}\sigma\right)^2 dv \\ &= \frac{1}{n}\sum_{k=0}^{n-1}\int_0^1\left(\frac{k^2}{n^2}a_k^2 + \frac{2k}{n^2}va_k\sigma + \frac{v^2}{n^2}\sigma^2\right)dv \\ &= \frac{1}{n}\sum_{k=0}^{n-1}\left(\frac{k^2}{n^2}a_k^2 + \frac{k}{n^2}a_k\sigma + \frac{\sigma^2}{3n^2}\right). \qquad (2.5)\end{aligned}$$

We postpone the estimation of $\mathbf{E}\,W_3^2$, and introduce the notation

$$b_n := \|W_3\|_2 = \|C_n(\lceil nU \rceil) - C(U)\|_2. \qquad (2.6)$$

Combining (2.3)–(2.6), we obtain our fundamental recursive estimate

$$\begin{aligned}a_n^2 &\le 2\mathbf{E}\,W_1^2 + \mathbf{E}\,W_3^2 \\ &\le \frac{2}{n^3}\sum_{k=1}^{n-1}k^2a_k^2 + \frac{2\sigma}{n^3}\sum_{k=1}^{n-1}ka_k + \frac{2\sigma^2}{3n^2} + b_n^2, \qquad n \ge 1. \qquad (2.7)\end{aligned}$$

We unwrap this recursion partly, by concentrating on the first sum on the right-hand side and regarding the second as known. Thus, writing

$$y_n := \frac{2\sigma}{n^3}\sum_{k=1}^{n-1}ka_k + \frac{2\sigma^2}{3n^2} + b_n^2, \qquad (2.8)$$

we define recursively

$$x_n := \frac{2}{n}\sum_{k=1}^{n-1}x_k + n^2y_n, \qquad n \ge 1, \qquad (2.9)$$

and find by (2.7) and induction

$$n^2a_n^2 \le x_n, \qquad n \ge 1.$$

Now, the recursion (2.9) is easily solved (see, e.g., [5]), giving

$$a_n^2 \le n^{-2}x_n = y_n + 2\frac{n+1}{n^2}\sum_{j=1}^{n-1}\frac{j^2}{(j+1)(j+2)}y_j, \qquad n \ge 1. \qquad (2.10)$$

We substitute (2.8), treating the three terms separately, into (2.10). The first term in (2.8) yields the sum

$$\begin{aligned}\sum_{j=1}^{n-1} \frac{j^2}{(j+1)(j+2)} \frac{2\sigma}{j^3} \sum_{k=1}^{j-1} ka_k &= \sum_{k=1}^{n-1} \sum_{k<j<n} \sigma k a_k \frac{2}{j(j+1)(j+2)} \\ &= \sum_{k=1}^{n-1} \sigma k a_k \sum_{j=k+1}^{n-1} \left(\frac{1}{j(j+1)} - \frac{1}{(j+1)(j+2)} \right) \\ &= \sum_{k=1}^{n-1} \sigma k a_k \left(\frac{1}{(k+1)(k+2)} - \frac{1}{n(n+1)} \right)\end{aligned}$$

and the total contribution

$$\begin{aligned}&\frac{2\sigma}{n^3} \sum_{k=1}^{n-1} ka_k + 2\frac{n+1}{n^2} \sum_{k=1}^{n-1} \sigma k a_k \left(\frac{1}{(k+1)(k+2)} - \frac{1}{n(n+1)} \right) \\ &\qquad = 2\sigma \frac{n+1}{n^2} \sum_{k=1}^{n-1} \frac{ka_k}{(k+1)(k+2)}. \qquad (2.11)\end{aligned}$$

The second term in (2.8) yields the sum

$$\sum_{j=1}^{n-1} \frac{j^2}{(j+1)(j+2)} \frac{2\sigma^2}{3j^2} = \frac{2\sigma^2}{3} \sum_{j=1}^{n-1} \left(\frac{1}{j+1} - \frac{1}{j+2} \right) = \frac{2\sigma^2}{3} \left(\frac{1}{2} - \frac{1}{n+1} \right)$$

and the total contribution

$$\frac{2\sigma^2}{3n^2} + 2\frac{n+1}{n^2} \frac{2\sigma^2}{3} \left(\frac{1}{2} - \frac{1}{n+1} \right) = \frac{2\sigma^2}{3n^2}(1+n+1-2) = \frac{2\sigma^2}{3n}. \qquad (2.12)$$

Hence we find from (2.10)

$$a_n^2 \le 2\sigma \frac{n+1}{n^2} \sum_{k=1}^{n-1} \frac{ka_k}{(k+1)(k+2)} + \frac{2\sigma^2}{3n} + b_n^2 + 2\frac{n+1}{n^2} \sum_{k=1}^{n-1} \frac{k^2 b_k^2}{(k+1)(k+2)}. \qquad (2.13)$$

We next use the following estimate of b_n, whose proof we postpone.

Lemma 2.2. *For $n \ge 1$,*

$$b_n := \|C_n(\lceil nU \rceil) - C(U)\|_2 \le \left(3 + \frac{2\pi}{\sqrt{3}} \right) \frac{1}{n} < \frac{6.63}{n}.$$

Using this lemma in (2.13), we find in analogy with (2.12)

$$b_n^2 + 2\frac{n+1}{n^2} \sum_{k=1}^{n-1} \frac{k^2 b_k^2}{(k+1)(k+2)} < \frac{(6.63)^2}{n} < \frac{44}{n} \qquad (2.14)$$

and thus

$$a_n^2 \le 2\sigma \frac{n+1}{n^2} \sum_{k=1}^{n-1} \frac{k a_k}{(k+1)(k+2)} + \left(44 + \frac{2\sigma^2}{3}\right)\frac{1}{n}, \qquad n \ge 1. \tag{2.15}$$

We claim that (2.15) implies the sought estimate $a_n = O(n^{-1/2})$. Indeed, assume that $n \ge 1$ and that $A > 0$ is a number such that

$$a_k \le A/\sqrt{k} \tag{2.16}$$

for $1 \le k \le n-1$. Then, using $k+1 \ge [k(k+2)]^{1/2}$,

$$\begin{aligned} \sum_{k=1}^{n-1} \frac{k a_k}{(k+1)(k+2)} &\le A \sum_{k=1}^{n-1} \frac{k^{1/2}}{(k+1)(k+2)} \le A \sum_{k=1}^{n-1} \frac{1}{(k+2)^{3/2}} \\ &\le A \int_0^{n-1} \frac{dx}{(x+2)^{3/2}} = 2A\left(2^{-1/2} - (n+1)^{-1/2}\right). \end{aligned} \tag{2.17}$$

In particular, for $n \ge 2$,

$$\frac{1}{n} \sum_{k=1}^{n-1} \frac{k a_k}{(k+1)(k+2)} \le \frac{1}{n} 2A \le 2A(n+1)^{-1/2} \tag{2.18}$$

and thus (2.17) yields (trivially for $n = 1$, too)

$$\frac{n+1}{n} \sum_{k=1}^{n-1} \frac{k a_k}{(k+1)(k+2)} \le 2^{1/2} A.$$

Consequently, by (2.15),

$$n a_n^2 \le 2^{3/2} \sigma A + 44 + 2\frac{\sigma^2}{3} \le 2^{3/2}\sigma A + 45.$$

If $2^{3/2}\sigma A + 45 \le A^2$, which holds for example for $A = 8$, then this yields $n a_n^2 \le A^2$, and thus (2.16) holds for $k = n$, too. By induction, (2.16) holds for all $k \ge 1$, and we have proved the explicit estimate

$$a_n \le \frac{8}{\sqrt{n}}, \qquad n \ge 1. \tag{2.19}$$

This is the desired estimate, apart from the value of the constant. To improve the constant, we use numerical calculations by computer. Indeed, for (2.6),

$$\begin{aligned} b_n^2 &= \sum_{i=1}^{n} \int_{(i-1)/n}^{i/n} (C(u) - C_n(i))^2 \, du \\ &= \int_0^1 C(u)^2 \, du - 2 \sum_{i=1}^{n} C_n(i) \int_{(i-1)/n}^{i/n} C(u) \, du + \sum_{i=1}^{n} \frac{1}{n} C_n(i)^2 \\ &= \frac{\sigma^2}{3} - 2 \sum_{i=1}^{n} C_n(i) \left(F\left(\frac{i}{n}\right) - F\left(\frac{i-1}{n}\right)\right) + \frac{1}{n} \sum_{i=1}^{n} C_n(i)^2, \end{aligned}$$

where $F(u) := u^2 \ln u - (1-u)^2 \ln(1-u)$ and $C_n(i)$ is given by (1.5); so, given any integer N, b_n can be computed exactly for $n \le N$. Next, for $n = 1, \dots, N$, an upper bound $\bar{a}_n$ to a_n can be computed recursively from (2.7) or, equivalently, (2.13), using the already computed $\bar{a}_k$, $k < n$, to bound a_k in the right-hand side. (We do not know how to compute a_n exactly even for $n = 3$.) For larger n, we use the estimates (2.16) and Lemma 2.2.

Let

$$\begin{aligned} V_n &:= \sum_{k=1}^{n} \frac{k a_k}{(k+1)(k+2)}, \\ \bar{V}_n &:= \sum_{k=1}^{n} \frac{k \bar{a}_k}{(k+1)(k+2)}, \\ W_n &:= \sum_{k=1}^{n} \frac{k^2 b_k^2}{(k+1)(k+2)}. \end{aligned}$$

Then for $n > N$, arguing as in (2.17), for any A such that (2.16) holds for all k,

$$V_{n-1} \le \bar{V}_N + \sum_{k=N+1}^{n-1} \frac{A}{(k+2)^{3/2}} \le \bar{V}_N + 2A\left((N+2)^{-1/2} - (n+1)^{-1/2}\right)$$

and thus by (2.18)

$$\tfrac{n+1}{n} V_{n-1} = V_{n-1} + \tfrac{1}{n} V_{n-1} \le \bar{V}_N + 2A(N+2)^{-1/2}. \tag{2.20}$$

Similarly, with $B := \left(3 + \frac{2\pi}{\sqrt{3}}\right)^2 < 44$, for $n > N$, by Lemma 2.2, we have

$$\begin{aligned} \tfrac{n+1}{n} W_{n-1} &\le W_N + \sum_{k=N+1}^{n-1} \frac{B}{(k+1)(k+2)} + \frac{1}{n} \sum_{k=1}^{n-1} \frac{B}{(k+1)(k+2)} \\ &= W_N + B\left(\frac{1}{N+2} - \frac{1}{n+1} + \frac{1}{2n} - \frac{1}{n(n+1)}\right) = W_N + \frac{B}{N+2} - \frac{B}{2n}. \end{aligned}$$

Consequently, (2.13) yields, using Lemma 2.2 again and (2.20),

$$\begin{aligned} a_n^2 &\le 2\sigma \frac{n+1}{n^2} V_{n-1} + \frac{2\sigma^2}{3n} + \frac{B}{n^2} + 2\frac{n+1}{n^2} W_{n-1} \\ &\le \frac{1}{n}\left(2\sigma \bar{V}_N + 4\sigma A(N+2)^{-1/2} + \frac{2\sigma^2}{3} + 2W_N + 2B(N+2)^{-1}\right), \qquad n > N. \end{aligned}$$

In other words, (2.16) holds for $k > N$, with A replaced by

$$A_N := \left(2\sigma \bar{V}_N + 4\sigma A(N+2)^{-1/2} + \frac{2\sigma^2}{3} + 2W_N + 2B(N+2)^{-1}\right)^{1/2}. \tag{2.21}$$

For $N = 100$ we find (using `Mathematica` or `Maple`), rounded to four decimal places, $\bar{V}_{100} \doteq 1.1995$ and $W_{100} \doteq 0.3466$, and thus, taking $A = 8$ as in (2.19), $A_{100} \doteq 2.3332$. Moreover, the computer verifies that $n^{1/2}\bar{a}_n < 1.7$ for $n \le 100$; thus (2.16) holds for all $k \ge 1$ with $A = 2.34$. Using this value in (2.21) we find $A_{100} \doteq 1.9976$, and the theorem is proved. $\square$

Remark 2.3. The sequence $n^{1/2}\bar{a}_n$ seems to increase slowly. For $n = 100$ the value is (rounded to four decimal places) 1.6018, and hence the bound in Theorem 2.1 cannot be much improved using the present method based on (2.7).

It remains to prove Lemma 2.2 above.

Proof of Lemma 2.2. Let $I_i := \{u : \lceil nu \rceil = i\} = ((i-1)/n, i/n]$. Thus $I_1, \dots, I_n$ form a partition of $(0, 1]$. We choose a point $t_i \in \bar{I}_i$ for each i (where the bar here indicates closure) and define

$$\tilde{C}_n(u) := C(t_{\lceil nu \rceil}),$$

i.e., $\tilde{C}(u) = C(t_i)$ when $u \in I_i$. By Minkowski's inequality,

$$b_n \le \|C_n(\lceil nU \rceil) - \tilde{C}_n(U)\|_2 + \|\tilde{C}_n(U) - C(U)\|_2. \tag{2.22}$$

To estimate the second term in (2.22), note that for $u \in I_i$,

$$|\tilde{C}_n(u) - C(u)| = |C(t_i) - C(u)| \le \int_{I_i} |C'(x)|\, dx.$$

The Cauchy–Schwarz inequality yields

$$|\tilde{C}_n(u) - C(u)|^2 \le \frac{1}{n} \int_{I_i} |C'(x)|^2\, dx, \qquad u \in I_i,$$

and thus (for any choice of $t_i \in \bar{I}_i$),

$$\begin{aligned} \|\tilde{C}_n(U) - C(U)\|_2^2 &= \sum_{i=1}^{n} \int_{I_i} |\tilde{C}_n(u) - C(u)|^2\, du \\ &\le \sum_{i=1}^{n} \frac{1}{n^2} \int_{I_i} |C'(x)|^2\, dx \\ &= \frac{1}{n^2} \int_0^1 |C'(x)|^2\, dx. \end{aligned} \tag{2.23}$$

We have

$$C'(x) = 2 \ln x - 2 \ln(1 - x)$$

and find

$$\int_0^1 [\ln(1-x)]^2\, dx = \int_0^1 (\ln x)^2\, dx = \int_0^\infty y^2 e^{-y}\, dy = 2$$

and

$$\begin{aligned} \int_0^1 [\ln x][\ln(1-x)]\, dx &= \sum_{k=1}^{\infty} \frac{1}{k} \int_0^1 x^k\, |\ln x|\, dx = \sum_{k=1}^{\infty} \frac{1}{k} \int_0^\infty e^{-ky} y e^{-y}\, dy \\ &= \sum_{k=1}^{\infty} \frac{1}{k} \frac{1}{(k+1)^2} = \sum_{k=1}^{\infty} \left(\frac{1}{k(k+1)} - \frac{1}{(k+1)^2} \right) \\ &= 1 - \left(\frac{\pi^2}{6} - 1 \right) = 2 - \frac{\pi^2}{6}; \end{aligned}$$

consequently,

$$\int_0^1 |C'(x)|^2\,dx = 8\int_0^1 (\ln x)^2\,dx - 8\int_0^1 [\ln x][\ln(1-x)]\,dx = \frac{4\pi^2}{3}.$$

Hence (2.23) yields

$$\|\tilde{C}_n(U) - C(U)\|_2 \le \frac{1}{n}\|C'(U)\|_2 \le \frac{2\pi}{\sqrt{3}n}. \tag{2.24}$$

For the first term in (2.22), let us first assume that $n \ge 2$. For $u \in I_i$ we have

$$\begin{aligned} C_n(\lceil nu\rceil) - \tilde{C}_n(u) &= C_n(i) - C(t_i) \\ &= -\tfrac{1}{n} + \tfrac{1}{n}(\mu_{i-1} + \mu_{n-i} - \mu_n) - 2t_i \ln t_i - 2(1-t_i)\ln(1-t_i). \end{aligned}$$

For $i \le \lceil n/2\rceil$ we choose $t_i = i/n$. This yields, using (1.11) and (1.10),

$$\begin{aligned} C_n(i) - C(t_i) &\le \tfrac{1}{n}\big[-1 + 2i\ln i + (2\gamma-4)i + 3 \\ &\qquad +2(n-i+1)\ln(n-i) + (2\gamma-4)(n-i) + 2\gamma + 1 + \tfrac{1}{n-i} \\ &\qquad -2(n+1)\ln n - (2\gamma-4)n - 2\gamma - 2i\ln(\tfrac{i}{n}) - 2(n-i)\ln(\tfrac{n-i}{n})\big] \\ &= \tfrac{1}{n}\left[2\ln(\tfrac{n-i}{n}) + 3 + \tfrac{1}{n-i}\right] \le \tfrac{1}{n}\left[3 - \tfrac{2i}{n} + \tfrac{1}{n-i}\right] \\ &\le \tfrac{3}{n}. \end{aligned} \tag{2.25}$$

In the opposite direction, by (1.11) and (1.10), still for $i \le \lceil n/2\rceil$,

$$\begin{aligned} C_n(i) - C(t_i) &\ge \tfrac{1}{n}\big[-1 + 2i\ln i + (2\gamma-4)i + 2 \\ &\qquad +2(n-i+1)\ln(n-i) + (2\gamma-4)(n-i) + 2\gamma \\ &\qquad -2(n+1)\ln n - (2\gamma-4)n - 2\gamma - 1 - \tfrac{1}{n} \\ &\qquad -2i\ln(\tfrac{i}{n}) - 2(n-i)\ln(\tfrac{n-i}{n})\big] \\ &= \tfrac{1}{n}\left[2\ln(\tfrac{n-i}{n}) - \tfrac{1}{n}\right] \ge \tfrac{1}{n}\left[2\ln(\tfrac{1}{3}) - \tfrac{1}{2}\right] \ge -\tfrac{3}{n}. \end{aligned}$$

Consequently, for $i \le \lceil n/2\rceil$,

$$|C_n(i) - C(t_i)| \le 3/n. \tag{2.26}$$

For $i > \lceil n/2\rceil$ we choose instead $t_i = (i-1)/n = 1 - t_{n+1-i}$. The symmetries of C_n and C then yield $C_n(i) - C(t_i) = C_n(n+1-i) - C(t_{n+1-i})$, and since $n+1-i \le n/2$, (2.26) shows that $|C_n(i) - C(t_i)| \le 3/n$ for $i > \lceil n/2\rceil$, too, i.e., (2.26) holds for all $i \le n$. In other words,

$$|C_n(\lceil nu\rceil) - \tilde{C}_n(u)| = |C_n(\lceil nu\rceil) - C(t_{\lceil nu\rceil})| \le 3/n$$

for all $u \in (0,1]$; in particular, $\|C_n(\lceil nU\rceil) - \tilde{C}_n(U)\|_2 \le 3/n$ for all $n \ge 2$. This holds trivially for $n = 1$, too, for any choice of t_1, and together with (2.22) and (2.24) yields the result. ∎

Remark 2.4. Define

$$c^* := \sup\{n^{1/2} d_2(Y_n, Y) : \ n \geq 1\},$$

so that, by Theorem 2.1, $c^* \leq 2$. Conversely,

$$c^* \geq 2^{1/2} d_2(Y_2, Y) = 2^{1/2} \|Y\|_2 = \sigma\sqrt{2} > 0.9168;$$

thus the constant 2 in Theorem 2.1 is no more than about twice the optimal value.

Although we do not know the exact value of $d_2(Y_n, Y)$ for any $n > 2$, one can in principle for any n and m compute the exact distributions of Y_n and Y_m and thus $d_2(Y_n, Y_m)$. We have done this for some $m, n \leq 50$ using `Mathematica` and `Maple`. The results are consistent with a decay of the type $d_2(Y_n, Y) \sim cn^{-1/2}$ with $c \approx 1$, but our data are too few to be conclusive.

3 Bounding $d_p(Y_n, Y)$

In this section we extend Theorem 2.1 and show that $d_p(Y_n, Y) = O(n^{-1/2})$ for every p. In contrast to the style of Section 2, we will make no attempt to keep constants small, nor to keep track of them explicitly.

Theorem 3.1. *For every $p \geq 1$, there exists a constant $c_p < \infty$ such that*

$$d_p(Y_n, Y) \leq c_p/\sqrt{n}, \qquad n \geq 1.$$

Proof. Since $d_p \leq d_q$ when $p \leq q$, it suffices to consider integer $p \geq 2$. The case $p = 2$ is Theorem 2.1 (with $c_2 = 2$), so we assume further that $p \geq 3$. We use induction on p and assume that the result holds for smaller positive integer values of p.

Let Y, Y_n, Y^*, Y_n^*, U be as in Section 2, and note that for every $p \geq 1$,

$$\|Y_n - Y\|_p = \|Y_n^* - Y^*\|_p = d_p(Y_n, Y), \qquad n \geq 0, \tag{3.1}$$

by the fact [1] that there is an optimal coupling for d_2 that is optimal for every d_p. Using the notation of Section 2, we have, for $n \geq 1$,

$$d_p(Y_n, Y) \leq \|\tilde{Y}_n - \tilde{Y}\|_p = \|W_1 + W_2 + W_3\|_p. \tag{3.2}$$

We use a simple lemma to estimate this.

Lemma 3.2. *Let Z_1, Z_2, and Z_3 be three independent random variables, and let $p \geq 2$ be an integer. Then*

$$\mathbf{E}\,|Z_1 + Z_2 + Z_3|^p \leq \mathbf{E}\,|Z_1|^p + \mathbf{E}\,|Z_2|^p + (\|Z_1\|_{p-1} + \|Z_2\|_{p-1} + \|Z_3\|_p)^p.$$

Proof. By the binomial theorem and independence,

$$\mathbf{E}\,|Z_1+Z_2+Z_3|^p \leq \mathbf{E}\,(|Z_1| + |Z_2| + |Z_3|)^p = \sum_{j,k,l} \binom{p}{j,k,l} \left(\mathbf{E}\,|Z_1|^j\right) \left(\mathbf{E}\,|Z_2|^k\right) \left(\mathbf{E}\,|Z_3|^l\right).$$

If $j \leq p-1$ and $k \leq p-1$ we estimate $\mathbf{E}\,|Z_1|^j = \|Z_1\|_j^j \leq \|Z_1\|_{p-1}^j$ (which holds also for $j=0$, disregarding the central expression) and similarly $\mathbf{E}\,|Z_2|^k \leq \|Z_2\|_{p-1}^k$ and $\mathbf{E}\,|Z_3|^l \leq \|Z_3\|_p^l$. Hence all terms in the sum, except $\mathbf{E}\,|Z_1|^p$ and $\mathbf{E}\,|Z_2|^p$, are bounded by the corresponding terms in the trinomial expansion of $(\|Z_1\|_{p-1} + \|Z_2\|_{p-1} + \|Z_3\|_p)^p$. □

Conditional on $U=u$, the three variables W_1, W_2, and W_3 are independent, so the lemma is applicable. Fix $u \in (0,1)$ and let $i = \lceil nu \rceil$, so $1 \leq i \leq n$. Then, given $U=u$, $W_1 = \frac{i-1}{n} Y_{i-1} - uY$ and thus, for any $q \geq 1$,

$$\begin{aligned}
\mathbf{E}\,(|W_1|^q \,|\, U=u)^{1/q} &= \|\tfrac{i-1}{n} Y_{i-1} - uY\|_q \\
&\leq \|\tfrac{i-1}{n}(Y_{i-1} - Y)\|_q + |\tfrac{i-1}{n} - u|\,\|Y\|_q \\
&\leq \tfrac{i-1}{n} d_q(Y_{i-1}, Y) + \tfrac{1}{n}\|Y\|_q. \qquad (3.3)
\end{aligned}$$

Similarly,

$$\mathbf{E}\,(|W_2|^q \,|\, U=u)^{1/q} \leq \tfrac{n-i}{n} d_q(Y_{n-i}, Y) + \tfrac{1}{n}\|Y\|_q. \qquad (3.4)$$

Further, given $U=u$, $W_3 = C_n(i) - C(u)$ is a constant, for which we use the simple estimate (from Proposition 3.2 in [19])

$$|W_3| = |C_n(\lceil nu \rceil) - C(u)| \leq \tfrac{6}{n} \ln n + O\left(n^{-1}\right) = O\left(n^{-1/2}\right). \qquad (3.5)$$

We first use (3.3) with $q = p-1$ together with the induction hypothesis $d_{p-1}(Y_{i-1}, Y) \leq c_{p-1}(i-1)^{-1/2}$, $i \geq 2$, to obtain (also for $i=1$)

$$\mathbf{E}\left(|W_1|^{p-1} \,|\, U=u\right)^{1/(p-1)} \leq c_{p-1}\frac{(i-1)^{1/2}}{n} + \frac{1}{n}\|Y\|_{p-1} \leq b_1 n^{-1/2},$$

where b_1, like b_2, b_3, b_4 below, denotes some constant depending on p only. By similar argument using (3.4) and (3.5), we obtain

$$\mathbf{E}\left(|W_1|^{p-1} \,|\, U=u\right)^{1/(p-1)} + \mathbf{E}\left(|W_2|^{p-1} \,|\, U=u\right)^{1/(p-1)} + \mathbf{E}\,(|W_3|^p \,|\, U=u)^{1/p} \leq b_2 n^{-1/2}.$$

Hence, using (3.3) and (3.4) for $q=p$, too, Lemma 3.2 yields

$$\begin{aligned}
\mathbf{E}\,(|W_1 + W_2 + W_3|^p \,|\, U=u) &\leq \left(\frac{i-1}{n} d_p(Y_{i-1}, Y) + b_3\frac{1}{n}\right)^p \\
&\quad + \left(\frac{n-i}{n} d_p(Y_{n-i}, Y) + b_3\frac{1}{n}\right)^p + b_2^p n^{-p/2}.
\end{aligned}$$

Taking the average over all $u \in (0,1)$ we finally find the recursive estimate

$$\begin{aligned}
d_p(Y_n, Y)^p &\leq \mathbf{E}\,|W_1 + W_2 + W_3|^p = \mathbf{E}\,\mathbf{E}\,(|W_1 + W_2 + W_3|^p \,|\, U) \\
&\leq \frac{2}{n}\sum_{j=0}^{n-1}\left(\frac{j}{n} d_p(Y_j, Y) + b_3\frac{1}{n}\right)^p + b_2^p n^{-p/2}. \qquad (3.6)
\end{aligned}$$

The proof is now completed by another induction, this one on n. Suppose that $d_p(Y_j, Y) \le cj^{-1/2}$ for $1 \le j \le n-1$. Then (3.6) yields

$$\begin{aligned} d_p(Y_n, Y)^p &\le \frac{2}{n}\sum_{j=1}^{n-1}\Bigl(cj^{1/2}n^{-1} + b_3 n^{-1}\Bigr)^p + \frac{2}{n}b_3^p n^{-p} + b_2^p n^{-p/2} \\ &\le \frac{2}{n}(c+b_3)^p \sum_{j=1}^{n-1} j^{p/2}n^{-p} + b_4 n^{-p/2} \\ &\le 2(c+b_3)^p \int_0^1 x^{p/2} n^{-p/2}\,dx + b_4 n^{-p/2} \\ &= \left[2(c+b_3)^p \frac{1}{(p/2)+1} + b_4\right] n^{-p/2}. \end{aligned} \tag{3.7}$$

Since $p \ge 3$, we have $\frac{2}{(p/2)+1} = \frac{4}{p+2} < 1$, and thus, if c is sufficiently large,

$$\frac{4}{p+2}(c+b_3)^p + b_4 \le c^p.$$

For such c, (3.7) yields $d_p(Y_n, Y)^p \le \bigl(cn^{-1/2}\bigr)^p$, which completes both inductions and the proof. ∎

Note that the arguments used above for $p \ge 3$ do not work for $p = 2$, so we need both the proof here and the proof in Section 2.

4 Lower bounds for $d_p(Y_n, Y)$

We do not know whether the upper bounds $O(n^{-1/2})$ proved in the preceding two sections are sharp. We give in this section two simple lower bounds.

First, $d_p(Y_n, Y) = \Omega(n^{-1})$ for every p by the following general result.

Proposition 4.1. *Let $W, W_1, W_2, \dots$ be random variables such that W has an absolutely continuous distribution while, for each $n \ge 1$ and some constant b_n, $n(W_n - b_n)$ is integer-valued. Then, for each $1 \le p < \infty$, $d_p(W_n, W) = \Omega(1/n)$. More precisely,*

$$\liminf_{n\to\infty} n\, d_p(W_n, W) \ge \tfrac{1}{2}(p+1)^{-1/p}. \tag{4.1}$$

Proof. Let $V_n := \{n(W - b_n)\}$, where $\{x\} := x - \lfloor x \rfloor$ denotes the fractional part of x. For any coupling of W and W_n,

$$|W - W_n| = \tfrac{1}{n}|n(W - b_n) - n(W_n - b_n)| \ge \tfrac{1}{n}h(V_n),$$

where $h(x) := \min(x, 1-x)$, $0 \le x \le 1$, and thus

$$d_p(W, W_n) \ge \tfrac{1}{n}\|h(V_n)\|_p. \tag{4.2}$$

We regard V_n as a random variable taking values in $\mathbf{R}/\mathbf{Z} \cong \mathbf{T}$, and find that its distribution, ν_n say, has Fourier coefficients

$$\hat{\nu}_n(k) = \mathbf{E}\left(e^{-2\pi i k V_n}\right) = e^{2\pi i k n b_n} \phi(-2\pi k n),$$

where ϕ is the characteristic function of W. In particular, $|\hat{\nu}_n(k)| = |\phi(2\pi k n)|$. By our hypothesis on W and the Riemann–Lebesgue lemma, $\phi(x) \to 0$ as $x \to \pm\infty$. Thus, for each fixed $k \neq 0$, $\hat{\nu}_n(k) \to 0$ as $n \to \infty$. This implies that ν_n converges weakly (as measures on $\mathbf{T}$) to the uniform distribution, i.e., $V_n \xrightarrow{\mathcal{L}} U$ where $U \sim \text{unif}(0,1)$. Consequently, as $n \to \infty$,

$$\|h(V_n)\|_p^p = \mathbf{E}\, h(V_n)^p \to \mathbf{E}\, h(U)^p = 2\int_0^{1/2} x^p \, dx = 2^{-p}/(p+1),$$

which together with (4.2) leads to (4.1). The proof of the proposition is completed by observing $d_p(W_n, W) > 0$ for every n, because $W_n \overset{\mathcal{L}}{\neq} W$. □

Note that, in contrast to the asymptotic result (4.1), there is no positive lower bound to $d_p(W_n, W)$ for a fixed n without further assumptions. Hence the implicit constant in $\Omega(1/n)$ in the theorem depends on the variables $W, W_1, \ldots$.

For $p \geq 2$ we can improve this lower bound by a logarithmic factor by using the known variance of Y_n.

Theorem 4.2. *If* $2 \leq p < \infty$, *then*

$$d_p(Y_n, Y) \geq d_2(Y_n, Y) = \Omega(\tfrac{\ln n}{n}).$$

Proof. Recall that Y and Y_n have mean 0 and that $\mathbf{Var}\, Y = \sigma^2$ while by (1.2)

$$\mathbf{Var}\, Y_n = \sigma^2 - 2\tfrac{\ln n}{n} + O(n^{-1})$$

and thus

$$\|Y_n\|_2 = (\mathbf{Var}\, Y_n)^{1/2} = \sigma - \tfrac{1}{\sigma}\tfrac{\ln n}{n} + O(n^{-1}).$$

Consequently, for the d_2-optimal coupling of Y and Y_n, by Minkowski's inequality,

$$d_2(Y_n, Y) = \|Y_n - Y\|_2 \geq \|Y\|_2 - \|Y_n\|_2 = \sigma^{-1}\tfrac{\ln n}{n} + O(n^{-1}).$$

□

We still have a gap between $(\ln n)/n$ and $n^{-1/2}$.

Remark 4.3. It can be shown that $\mathbf{E}\, Y_n^m = \mathbf{E}\, Y^m + O\left(\frac{\ln n}{n}\right)$, $n \geq 2$, holds also for $m = 3, 4, \ldots$; cf. the formulas for moments and cumulants by Hennequin [11]. Hence we do not get better lower bounds for d_p by considering higher moments.

5 The Kolmogorov–Smirnov distance

Recall that the Kolmogorov–Smirnov distance $d_{\mathrm{KS}}(F, G)$ between two distributions is defined as $\sup_{x\in\mathbf{R}} |P(X \le x) - P(Y \le x)|$, when $X \sim F$ and $Y \sim G$. We will in this case also write $d_{\mathrm{KS}}(X, Y)$.

To obtain upper bounds for $d_{\mathrm{KS}}(Y_n, Y)$, we combine the bounds above for $d_p(Y_n, Y)$ with the following simple general result and the fact [6] that Y has a bounded density function.

Lemma 5.1. *Suppose that X and Y are two random variables such that Y is absolutely continuous with a bounded density function f. If $M := \sup_{y\in\mathbf{R}} |f(y)|$ and $1 \le p < \infty$, then*

$$d_{\mathrm{KS}}(X, Y) \le (p+1)^{1/(p+1)} \left(M d_p(X, Y)\right)^{p/(p+1)}.$$

Proof. Consider an optimal d_p-coupling of X and Y. Then, for $x \in \mathbf{R}$ and $\varepsilon > 0$, denoting the distribution functions of X and Y by F_X and F_Y,

$$\begin{aligned} F_X(x) = P(X \le x) &\le P(Y \le x) + P(x < Y \le x+\varepsilon) + P(Y - X > \varepsilon) \\ &\le F_Y(x) + M\varepsilon + P(Y - X > \varepsilon). \end{aligned}$$

Similarly,

$$\begin{aligned} F_Y(x) &\le P(X \le x) + P(x-\varepsilon < Y \le x) + P(X - Y > \varepsilon) \\ &\le F_X(x) + M\varepsilon + P(X - Y > \varepsilon). \end{aligned}$$

Consequently,

$$\Delta(x) := |F_X(x) - F_Y(x)| \le M\varepsilon + P(|X - Y| > \varepsilon)$$

and thus

$$\begin{aligned} d_p(X, Y)^p = \mathbf{E}\,|X - Y|^p &= \int_0^\infty p\varepsilon^{p-1} P(|X - Y| > \varepsilon)\, d\varepsilon \\ &\ge \int_0^{\Delta(x)/M} p\varepsilon^{p-1}(\Delta(x) - M\varepsilon)\, d\varepsilon \\ &= \tfrac{1}{p+1}\Delta(x)^{p+1} M^{-p}. \end{aligned}$$

□

Theorem 5.2. *For every $\varepsilon > 0$,*

$$d_{\mathrm{KS}}(Y_n, Y) = O\left(n^{\varepsilon-(1/2)}\right).$$

Proof. By [6], Y has a bounded density function, so Lemma 5.1 and Theorem 3.1 yield, for every fixed $1 \le p < \infty$,

$$d_{\mathrm{KS}}(Y_n, Y) = O\left(d_p(Y_n, Y)^{p/(p+1)}\right) = O\left(n^{-p/[2(p+1)]}\right).$$

The result follows by choosing p so large that $\frac{p}{2(p+1)} > \frac{1}{2} - \varepsilon$. □

To get an explicit bound we take $p = 2$ in Lemma 5.1 and use Theorem 2.1. This yields the bound $3^{1/3}\left(2Mn^{-1/2}\right)^{2/3}$, and we know $M < 16$ from Theorem 3.3 of [6]. Hence,

Theorem 5.3. *For $n \geq 1$,*

$$d_{\mathrm{KS}}(Y_n, Y) \leq (12M^2)^{1/3} n^{-1/3} < (3072/n)^{1/3} < 15\, n^{-1/3}. \quad \square$$

Numerical evidence [20] suggests that $M < 1$, which would give a bound $2.3\, n^{-1/3}$.

As stated in the introduction, we do not know the right order of decay. The rate $O(n^{\varepsilon - 1/2})$ in Theorem 5.2 can be marginally improved to $\exp(C\sqrt{\ln n})n^{-1/2}$ by checking that the proof of Theorem 3.1 yields $c_p = O(c^p)$ for some c and then choosing $p = (\ln n)^{1/2}$ in Lemma 5.1. We omit the details, since it is likely that this still is far from the truth.

The best lower bound we can prove is $\Omega(n^{-1})$.

Theorem 5.4.

$$d_{\mathrm{KS}}(Y_n, Y) > \frac{1}{8(n+1)}, \qquad n \geq 1.$$

Again, the lower bound follows from quite general considerations. In this case we use the following lemma.

Lemma 5.5. *Suppose that Y and Z are two random variables such that Y has a continuous distribution while $a(Z - b)$ is integer-valued for some real numbers $a > 0$ and b. If $\sigma_Z^2 := \mathbf{Var}\, Z < \infty$, then*

$$d_{\mathrm{KS}}(Y, Z) \geq 1/(12a\sigma_Z + 8).$$

Proof. For any $x \in \mathbf{R}$ and $\delta > 0$,

$$F_Z(x+\delta) - F_Y(x+\delta) + F_Y(x-\delta) - F_Z(x-\delta) \leq 2d_{\mathrm{KS}}(Y, Z).$$

Letting $\delta \to 0$ we find, since Y is continuous,

$$P(Z = x) \leq 2d_{\mathrm{KS}}(Y, Z).$$

The result now follows from the following lemma applied to $a(Z - b)$. $\square$

Lemma 5.6. *If Z is an integer-valued random variable with finite variance σ_Z^2, then*

$$\sup_n P(Z = n) \geq 1/(6\sigma_Z + 4).$$

Proof. Let $\mu := \mathbf{E}\, Z$ and $m := \left\lceil \frac{3}{2}\sigma_Z \right\rceil$. By Chebyshev's inequality,

$$P(|Z - \mu| \geq m) \leq \frac{\sigma_Z^2}{m^2} \leq \frac{4}{9} < \frac{1}{2}$$

and thus

$$P(\mu - m < Z < \mu + m) > 1/2.$$

The interval $(\mu - m, \mu + m)$ contains at most $2m$ integers, and thus it must contain an integer n such that

$$P(Z = n) \geq \frac{1}{2m} P(\mu - m < Z < \mu + m) > \frac{1}{4m} > \frac{1}{6\sigma_Z + 4}. \quad \square$$

Proof of Theorem 5.4. We apply Lemma 5.5 with $a = n$ and observe that

$$\sigma_{Y_n} := (\mathbf{Var}\, Y_n)^{1/2} < \sigma = (\mathbf{Var}\, Y)^{1/2} \tag{5.1}$$

and that $12\sigma \doteq 7.8 < 8$. Indeed, (5.1) is trivial for $n = 1$ or 2 and easily verified for $3 \le n \le 6$, while for $n \ge 7$ it holds because then, by (1.2) and (1.3),

$$\begin{aligned}
\sigma^2 - \mathbf{Var}\, Y_n &= -4\frac{\pi^2}{6} + 4\left(1 + \frac{1}{n}\right)^2 H_n^{(2)} + 2\frac{n+1}{n^2} H_n - \frac{13}{n} \\
&> -4 \sum_{k=n+1}^{\infty} k^{-2} + \frac{8}{n} H_n^{(2)} + \frac{2}{n} H_n - \frac{13}{n} \\
&> \tfrac{1}{n}\left(-4 + 8H_n^{(2)} + 2H_n - 13\right) > 0.
\end{aligned}$$

□

6 Approximating the density of Y

It was shown in [6] that the density f of Y is infinitely differentiable, with all derivatives rapidly decaying. In particular, the derivative f' is bounded; Theorem 3.3 of [6] gives the explicit bound

$$M' := \sup_{x \in \mathbf{R}} |f'(x)| < 2466.$$

(This is not very sharp; the true value seems to be less than 2.) The bounds above on the Kolmogorov–Smirnov distance then imply the following local result.

Theorem 6.1. *For any $x \in \mathbf{R}$ and $\delta > 0$,*

$$\left| \frac{F_n(x + \frac{\delta}{2}) - F_n(x - \frac{\delta}{2})}{\delta} - f(x) \right| \le \frac{(96M^2)^{1/3}}{\delta n^{1/3}} + \frac{M'}{4}\delta.$$

In particular, for any $\bar{M} \ge M$ and $\bar{M}' \ge M'$, choosing $\delta = \delta_n := 2\left(96\bar{M}^2(\bar{M}')^{-3}\right)^{1/6} n^{-1/6}$ yields

$$\left| \frac{F_n(x + \frac{\delta_n}{2}) - F_n(x - \frac{\delta_n}{2})}{\delta_n} - f(x) \right| \le \left(96\bar{M}^2(\bar{M}')^3\right)^{1/6} n^{-1/6}. \tag{6.1}$$

The choices $\bar{M} = 16$ and $\bar{M}' = 2466$ provided by [6] yield the bound $268\, n^{-1/6}$ in (6.1). If $\bar{M} = 1$ and $\bar{M}' = 2$ could be proven to be legitimate, we could reduce the bound to $3.03\, n^{-1/6}$.

Proof. By Theorem 5.3,

$$\left|F_n\left(x + \tfrac{\delta}{2}\right) - F_n\left(x - \tfrac{\delta}{2}\right) - \left(F\left(x + \tfrac{\delta}{2}\right) - F\left(x - \tfrac{\delta}{2}\right)\right)\right| \le 2d_{\mathrm{KS}}(Y_n, Y) \le 2(12M^2)^{1/3} n^{-1/3},$$

while

$$\begin{aligned}
\left| F\left(x + \frac{\delta}{2}\right) - F\left(x - \frac{\delta}{2}\right) - \delta f(x) \right| &= \left| \int_{-\delta/2}^{\delta/2} (f(x+y) - f(x))\, dy \right| \\
&\le \int_{-\delta/2}^{\delta/2} M'|y|\, dy = \frac{M'}{4}\delta^2.
\end{aligned}$$

The first estimate follows, and the second is an immediate consequence. □

Theorem 6.1 yields a simple method to numerically calculate the unknown density f up to any given accuracy. For an application, see [2]. (In [2], a preliminary version of Theorem 6.1 with larger constants is used.) Note, however, that the convergence is slow and that it seems impractical to obtain high precision by this method. Other, potentially more powerful, methods to calculate f numerically are discussed in [8].

Open Problem 6.2. Does a local limit theorem hold in the form that

$$\left|nP(X_n = k) - f\left(\frac{k-\mu_n}{n}\right)\right| = \left|nP\left(Y_n = \frac{k-\mu_n}{n}\right) - f\left(\frac{k-\mu_n}{n}\right)\right| \to 0,$$

perhaps uniformly in $k \in \mathbf{Z}$, as $n \to \infty$?

7 Bounds on moment generating functions

Rösler [19] proved that the moment generating functions $\mathbf{E}\, e^{\lambda Y_n}$ are bounded for fixed λ, and thus $\mathbf{E}\, e^{\lambda Y_n} \to \mathbf{E}\, e^{\lambda Y}$ as $n \to \infty$. Rösler did not make his estimates explicit, but his method can be used to obtain explicit bounds. For the limit variable Y, this was done in [8], where we obtained by Rösler's method (with some refinements) the following explicit estimates for the moment generating function of Y: Let $L_0 \doteq 5.018$ be the largest root of $e^L = 6L^2$; then

$$\psi_Y(\lambda) := \mathbf{E}\, e^{\lambda Y} \le \begin{cases} e^{1.25\lambda^2}, & \lambda \le -0.62, \\ e^{0.5\lambda^2}, & -0.62 \le \lambda \le 0, \\ e^{\lambda^2}, & 0 \le \lambda \le 0.42, \\ e^{12\lambda^2}, & 0.42 \le \lambda \le L_0, \\ e^{2e^\lambda}, & L_0 \le \lambda. \end{cases} \tag{7.1}$$

In particular, $\mathbf{E}\, e^{\lambda Y} \le \exp\left(\max\left(12\lambda^2, 2e^\lambda\right)\right)$ for all $\lambda \in \mathbf{R}$.

The constants in (7.1) are not sharp, but the doubly exponential growth as $\lambda \to +\infty$ is correct: it was also shown in [8] that $\psi_Y(\lambda) \ge \exp\left(\gamma\lambda^{-1}e^\lambda\right)$ for all large λ whenever $\gamma < 2/e$.

In this section we will establish similar bounds for $\mathbf{E}\, e^{\lambda Y_n}$. For simplicity we first consider the slight shrinkage

$$\hat{Y}_n := \frac{n}{n+1} Y_n = \frac{X_n - \mu_n}{n+1}$$

of Y_n; in particular, $\hat{Y}_0 := X_0 - \mu_0 = 0$. We then have the following simple result.

Theorem 7.1. $\mathbf{E}\, e^{\lambda \hat{Y}_n} \uparrow \mathbf{E}\, e^{\lambda Y}$ *as* $n \uparrow \infty$. *Hence, for any* $n \ge 0$, $\mathbf{E}\, e^{\lambda \hat{Y}_n} \le \mathbf{E}\, e^{\lambda Y}$, *and in particular the upper bounds on* $\mathbf{E}\, e^{\lambda Y}$ *in* (7.1) *above apply also to* $\mathbf{E}\, e^{\lambda \hat{Y}_n}$.

Proof. It is well known that the number X_n of `Quicksort` comparisons has the same distribution as the internal path length of a random binary search tree (under the random permutation model) with n internal nodes—see, e.g., [15, Section 6.2.2]. Moreover, it was shown by Régnier [18] that when X_n is reinterpreted as the internal path length of an evolving random binary search tree after n keys have been inserted, the process $(\hat{Y}_n)_{n\geq 0}$ is a martingale, which is L^2-bounded and thus converges a.s. and in L^2 to some limit Y. It follows that also $Y_n \to Y$ a.s., and thus in distribution; hence this random variable Y is (a realization of) the same Y as above.

The martingale property can be written $\hat{Y}_n = \mathbf{E}\,(\hat{Y}_{n+1}|\mathcal{F}_n)$, for the appropriate σ-field $\mathcal{F}_n$. Since $x \mapsto e^{\lambda x}$ is convex, it now follows by Jensen's inequality for conditional expectations that $e^{\lambda \hat{Y}_n} \leq \mathbf{E}\,(e^{\lambda \hat{Y}_{n+1}}|\mathcal{F}_n)$; and thus, taking expectations, $\mathbf{E}\,e^{\lambda \hat{Y}_n} \leq \mathbf{E}\,e^{\lambda \hat{Y}_{n+1}}$.

By the same argument, $\mathbf{E}\,e^{\lambda \hat{Y}_n} \leq \mathbf{E}\,e^{\lambda Y}$ for each $n \geq 0$, which together with Fatou's lemma yields $\mathbf{E}\,e^{\lambda \hat{Y}_n} \to \mathbf{E}\,e^{\lambda Y}$ as $n \to \infty$. □

Corollary 7.2. *For every $n \geq 1$, we have*

$$\mathbf{E}\,e^{\lambda Y_n} \leq \begin{cases} e^{1.25[1+(1/n)]^2\lambda^2}, & \lambda \leq 0, \\ e^{0.5[1+(1/n)]^2\lambda^2}, & -0.62\,n/(n+1) \leq \lambda \leq 0, \\ e^{[1+(1/n)]^2\lambda^2}, & 0 \leq \lambda \leq 0.42\,n/(n+1), \\ e^{12[1+(1/n)]^2\lambda^2}, & 0 \leq \lambda \leq L_0\,n/(n+1), \\ e^{2e^{[1+(1/n)]\lambda}}, & L_0\,n/(n+1) \leq \lambda. \end{cases}$$

In particular, $\mathbf{E}\,e^{\lambda Y_n} \leq \exp\left(\max\left(12[1+(1/n)]^2\lambda^2, 2e^{[1+(1/n)]\lambda}\right)\right)$ *for all* $\lambda \in \mathbf{R}$.

Proof. $\lambda Y_n = \lambda_n \hat{Y}_n$ with $\lambda_n := [1+(1/n)]\lambda$. □

Remark 7.3. The factors $[1+(1/n)]$ in Corollary 7.2 are annoying but hardly important in applications. With some effort, we have been able to modify the proof in [8] and obtain for $\lambda \geq -0.58$ the same estimates for $\mathbf{E}\,e^{\lambda Y_n}$ as obtained there for $\mathbf{E}\,e^{\lambda Y}$; for $\lambda < -0.58$ we only obtain a slightly weaker bound, which for large n is inferior to the bound in Corollary 7.2. More precisely, we have shown

$$\mathbf{E}\,e^{\lambda Y_n} \leq \begin{cases} e^{1.34\lambda^2}, & \lambda \leq -0.58, \\ e^{0.5\lambda^2}, & -0.58 \leq \lambda \leq 0, \\ e^{\lambda^2}, & 0 \leq \lambda \leq 0.42, \\ e^{12\lambda^2}, & 0.42 \leq \lambda \leq L_0, \\ e^{2e^{\lambda}}, & L_0 \leq \lambda. \end{cases} \tag{7.2}$$

In particular, $\mathbf{E}\,e^{\lambda Y_n} \leq \exp\left(\max\left(12\lambda^2, 2e^{\lambda}\right)\right)$ for all $\lambda \in \mathbf{R}$. In other words, we can eliminate the factors $[1+(1/n)]$ in Corollary 7.2 for $\lambda \geq -0.58$ (and in particular for all positive λ). Since the proof is quite long and the result only marginally improves Corollary 7.2, we give the proof not here but rather in a separate appendix [9].

It seems likely that with further effort one could remove the factor $[1+(1/n)]$ for $\lambda < -0.58$ too, so that all the bounds in (7.1) also would bound $e^{\lambda Y_n}$. Moreover, it seems quite likely that $\mathbf{E}\, e^{\lambda Y_n} \le \mathbf{E}\, e^{\lambda Y}$ holds for all λ and n, and perhaps even that $\mathbf{E}\, e^{\lambda Y_n} \uparrow \mathbf{E}\, e^{\lambda Y}$, as was proved for $\hat{Y}_n$ in Theorem 7.1.

Theorem 7.1 enables us to get an explicit constant in Rösler's [19] large deviation bound.

Corollary 7.4. *For any $\varepsilon > 0$ and $\lambda > 0$,*

$$P(|X_n - \mu_n| \ge \varepsilon\mu_n) \le 2\exp\left[3\varepsilon\lambda + \max\left(12\lambda^2, 2e^{\lambda}\right)\right] n^{-2\varepsilon\lambda}.$$

Proof. By Markov's inequality,

$$\begin{aligned} P(|X_n - \mu_n| \ge \varepsilon\mu_n) &= P(|\hat{Y}_n| \ge \varepsilon\mu_n/(n+1)) \\ &\le \exp(-\varepsilon\lambda\mu_n/(n+1))\mathbf{E}\, e^{\lambda|\hat{Y}_n|} \\ &\le \exp(-\varepsilon\lambda\mu_n/(n+1))\left(\mathbf{E}\, e^{\lambda\hat{Y}_n} + \mathbf{E}\, e^{-\lambda\hat{Y}_n}\right). \end{aligned}$$

The result follows from Theorem 7.1, since $\mu_n/(n+1) \ge 2H_n - 4 \ge 2\ln n - 3$ by (1.7) and (1.9). □

Corollary 7.5. *For any fixed $\varepsilon > 0$,*

$$P(|X_n - \mu_n| \ge \varepsilon\mu_n) \le n^{-2\varepsilon \ln\ln n + O(1)}, \qquad n \ge 2.$$

Proof. Take (for $n \ge 3$) $\lambda = \ln\ln n$ in Corollary 7.4. □

The bound in Corollary 7.5 is essentially the same as the one obtained by McDiarmid and Hayward [16] by different methods; the only difference is a slight improvement in the error term. More generally, McDiarmid and Hayward [16] considered ε varying with n such that $1/\ln n < \varepsilon \le 1$; if we take $\lambda = \ln\ln n + \ln\varepsilon$ in Corollary 7.4, we obtain the bound in their Theorem 1.1 with $O(\ln\ln\ln n)$ improved to $O(1)$. Compare also the related large deviation estimates for the limit distribution Y in [8] (by similar arguments) and Knessl and Szpankowski [13] (much more precise, but assuming an as yet unverified regularity hypothesis).

Finally we show that the rate of convergence of the moment generating functions $\mathbf{E}\, e^{\lambda Y_n}$ to $\mathbf{E}\, e^{\lambda Y}$ also is $O(n^{-1/2})$. (The same holds for $\mathbf{E}\, e^{\lambda\hat{Y}_n}$.)

Theorem 7.6. *For any fixed complex λ,*

$$\mathbf{E}\, e^{\lambda Y_n} = \mathbf{E}\, e^{\lambda Y} + O(n^{-1/2}).$$

Explicitly, with $\lambda_1 := \mathrm{Re}(\lambda)$,

$$\left|\mathbf{E}\, e^{\lambda Y_n} - \mathbf{E}\, e^{\lambda Y}\right| \le 3|\lambda|\exp\left[\max\left(24[1+(1/n)]^2\lambda_1^2, e^{2[1+(1/n)]\lambda_1}\right)\right] n^{-1/2}.$$

Proof. Consider a d_2-optimal coupling of Y_n and Y. Then, using the mean value theorem, the Cauchy–Schwarz inequality, Corollary 7.2, and (7.1),

$$\begin{aligned}
\left|\mathbf{E}\, e^{\lambda Y_n} - \mathbf{E}\, e^{\lambda Y}\right| &\leq \mathbf{E}\left|e^{\lambda Y_n} - e^{\lambda Y}\right| \\
&\leq \mathbf{E}\left(|\lambda||Y_n - Y|\, e^{\max(\lambda_1 Y_n, \lambda_1 Y)}\right) \\
&\leq |\lambda| \left(\mathbf{E}\,|Y_n - Y|^2\right)^{1/2} \left(\mathbf{E}\, e^{2\max(\lambda_1 Y_n, \lambda_1 Y)}\right)^{1/2} \\
&\leq |\lambda| d_2(Y_n, Y) \left(\mathbf{E}\, e^{2\lambda_1 Y_n} + \mathbf{E}\, e^{2\lambda_1 Y}\right)^{1/2} \\
&\leq \sqrt{2}\,|\lambda| \exp\left[\max\left(24[1 + (1/n)]^2 \lambda_1^2, e^{2[1+(1/n)]\lambda_1}\right)\right] d_2(Y_n, Y).
\end{aligned}$$

The result follws by Theorem 2.1. ◻

Remark 7.7. By Remark 7.3, the factors $[1+(1/n)]$ can be eliminated in the statement of Theorem 7.6.

Acknowledgment. We thank Anhua Lin and Ludger Rüschendorf for helpful discussions. We also thank two anonymous referees for useful suggestions.

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