Appendix to Quicksort Asymptotics

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ABSTRACT

This appendix to [2] contains a proof of the improved estimates in Remark 7.3 of that paper for the moment generating function of the (normalized) number of comparisons in Quicksort.

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This is an appendix to [2], to which we refer for background and notation. The theorem, lemmas, and equations in this appendix are labelled by A.1, etc.; labels with pure numbers refer to [2].

The purpose of this appendix is to provide a proof of the following estimates stated in Remark 7.3 of [2].

Theorem A.1. Let $L_0 \doteq 5.018$ be the largest root of $e^L = 6L^2$. Then, for all $n \ge 0$,

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

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

The proof below follows closely the corresponding proof in [1], where we obtained by the method of Rösler [3] (with some refinements) explicit estimates for the moment generating function of the limit variable Y. In this appendix we treat instead the normalized number of comparisons Y_n for finite n. In the present case, some estimates involving $C_n(i)$, stated as lemmas below, become harder than the corresponding estimates in [1] where the limit as $n \to \infty$ is treated. Note that the bound in Theorem A.1 is the same as the one obtained for $\mathbf{E} e^{\lambda Y}$ in [1] for $\lambda \ge 0$, but slightly weaker for $\lambda < 0$ (or rather for $\lambda < -0.58$). (It seems likely that with further effort one could show that the bounds in [1] for $\mathbf{E} e^{\lambda Y}$ hold also for $\mathbf{E} e^{\lambda Y_n}$ for all λ and n, but this is still an open problem.)

In order to obtain good estimates we use extensive numerical calculations for small n to supplement our analytical estimates; we could do without these numerical calculations at the cost of increasing the constants in the exponents in the theorem. [All numerical calculations have been verified independently by the two authors, the (alphabetically) first using Mathematica and the second using Maple.]

We begin with some estimates of $C_n(i)$.

Lemma A.2. The sequence $(\mu_n)_{n\geq 0}$ is nondecreasing and convex.

Proof. By (1.7) and (1.8), for $n \ge 0$,

$$\mu_{n+1} - \mu_n = 2(n+2)H_{n+1} - 4(n+1) - [2(n+1)H_{n+1} - 4(n+1) + 2]$$

= 2H_{n+1} - 2, (A.1)

which is nonnegative and increasing.

Lemma A.3. For every $n \ge 1$, the sequence $(C_n(i))_{1 \le i \le n}$ is convex. Its maximum is $C_n(1) = C_n(n)$ and its minimum is $C_n(\lfloor (n+1)/2 \rfloor) = C_n(\lceil (n+1)/2 \rceil)$.

Proof. The definition (1.5) and Lemma A.2 show that $(C_n(i))_{1 \le i \le n}$ is convex. Moreover, $C_n(i) \equiv C_n(n+1-i)$, and the result follows.

Lemma A.4. If $1 \le i \le n$, then

$$-\eta \le C_n(i) \le 1,$$

where $\eta := 2 \ln 2 - 1 \doteq 0.3863$.

Proof. By Lemma A.3 and (1.5)

$$C_n(i) \le C_n(1) = \frac{1}{n}(n-1+\mu_0+\mu_{n-1}-\mu_n) \le \frac{n-1}{n} \le 1,$$

because $\mu_0 = 0$ and $\mu_{n-1} \leq \mu_n$ by Lemma A.2.

For the lower bound we first consider n odd, n = 2m - 1 with $m \ge 1$. By Lemma A.3, (1.5), and (1.8),

$$C_{2m-1}(i) \geq C_{2m-1}(m) = \frac{1}{2m-1}(2m-2+\mu_{m-1}+\mu_{m-1}-\mu_{2m-1})$$

= $\frac{1}{2m-1}[2m-2+2(2mH_m-4m+2)-(4mH_{2m}-8m+2)]$
= $\frac{2m}{2m-1}(1+2H_m-2H_{2m}).$ (A.2)

Note that for $k \ge 2$ we have $\ln k - \ln(k-1) = -\ln(1-\frac{1}{k}) > \frac{1}{k} + \frac{1}{2k^2}$, and thus

$$\delta_m := 2\ln 2 + 2(H_m - H_{2m}) = 2\sum_{k=m+1}^{2m} \left(\ln k - \ln(k-1) - \frac{1}{k}\right)$$

>
$$\sum_{k=m+1}^{2m} \frac{2}{2k^2} > \sum_{k=m+1}^{2m} \left(\frac{1}{k} - \frac{1}{k+1}\right) = \frac{1}{m+1} - \frac{1}{2m+1} = \frac{m}{(m+1)(2m+1)}.$$

Hence, if $m \geq 2$, then

$$2m\delta_m = \frac{2m^2}{(m+1)(2m+1)} \ge \frac{8}{15} > \eta,$$

while if m = 1, then $\delta_1 = \eta$. Therefore,

$$-C_{2m-1}(i) \le -C_{2m-1}(m) = \frac{2m}{2m-1}(-1+2\ln 2 - \delta_m) < \frac{2m}{2m-1}\left(\eta - \frac{\eta}{2m}\right) = \eta.$$

If n = 2m is even, then Lemma A.3, (1.5), (1.7), and (1.8) similarly yield

$$C_{2m}(i) \geq C_{2m}(m) = \frac{1}{2m}(2m - 1 + \mu_{m-1} + \mu_m - \mu_{2m})$$

= $\frac{1}{2m}[2m - 1 + 2mH_m - 4m + 2 + 2(m+1)H_m - 4m - (2(2m+1)H_{2m} - 8m)]$
= $\frac{2m+1}{2m}(1 + 2H_m - 2H_{2m}).$

Comparing with (A.2) we find by the estimate above $|C_{2m}(m)| < |C_{2m-1}(m)| < \eta$, and the result follows.

Lemma A.5. For $n \ge 1$ and $U_n \sim \text{unif}\{1, \ldots, n\}$, the sequence $\mathbf{E} C_n(U_n)^2$ is strictly increasing, and therefore

$$\mathbf{E} C_n(U_n)^2 = \frac{1}{n} \sum_{i=1}^n C_n(i)^2 < \mathbf{E} C(U)^2 = \sigma^2/3 \doteq 0.140.$$

Proof. We could use Lemma 2.2, Minkowski's inequality, and numerical calculations by computer to verify $\mathbf{E} C_n(U_n) < 0.15$, but we can do slightly better. Indeed, from the results in Section 1, one obtains the formula

$$\mathbf{E} C_n (U_n)^2 = \frac{7}{3} \left(1 + \frac{1}{n} \right)^2 - \frac{4}{3} \left(1 + \frac{2}{n} \right) \left(1 + \frac{1}{n} \right) H_n^{(2)} - \frac{4}{3} n^{-3} H_n, \qquad n \ge 1.$$

From this expression it is simple (if somewhat laborious) to prove increasingness. Finally, the limiting value of $\mathbf{E} C_n(U_n)^2$ is $\mathbf{E} C(U)^2 = \sigma^2/3$.

Lemma A.6. For $1 \le i \le n$,

$$C_n(i) - 2\eta \left[\left(\frac{i-1}{n} \right)^2 + \left(\frac{n-i}{n} \right)^2 - 1 \right] \ge 0.$$

Proof. Fix n and denote the left-hand side by x_i . By (1.5) and (A.1), for $1 \le i \le n-1$ we have

$$n^{2}(x_{i+1} - x_{i}) = n(\mu_{i} - \mu_{i-1} + \mu_{n-i-1} - \mu_{n-i}) + 2\eta \left[(i-1)^{2} - i^{2} + (n-i)^{2} - (n-i-1)^{2} \right] = 2nH_{i} - 2nH_{n-i} + 2\eta(2n-4i)$$

and thus, for $1 \le i \le n-2$,

$$n^{2}(x_{i+2} - 2x_{i+1} + x_{i}) = \frac{2n}{i+1} + \frac{2n}{n-i} - 8\eta = \frac{2n(n+1)}{(i+1)(n-i)} - 8\eta \ge \frac{2n(n+1)}{[(n+1)/2]^{2}} - 8\eta$$
$$= \frac{8n}{n+1} - 8\eta \ge 4 - 8\eta > 0.$$

Hence $(x_i)_{1 \le i \le n}$ is convex. Moreover $x_i = x_{n+1-i}$, and thus the minimum is x_{i_0} with $i_0 = \lfloor (n+1)/2 \rfloor$. Since $i_0 - 1 \le n/2 \le i_0$,

$$2\eta \left[\left(\frac{i_0 - 1}{n}\right)^2 + \left(\frac{n - i_0}{n}\right)^2 - 1 \right] \le 2\eta \left(\frac{1}{4} + \frac{1}{4} - 1\right) = -\eta \le C_n(i_0)$$

by Lemma A.4. Hence $x_{i_0} \ge 0$ and the result follows.

Lemma A.7. If $1 \le i \le n$ and $(i-1)/n \le u \le i/n$, then

$$u(1-u)C_n(i) \le 0.05.$$

Proof. The left-hand side is not changed if we replace i by n + 1 - i and u by 1 - u; hence we may assume that $i \leq (n+1)/2$. Moreover if n is odd and i = (n+1)/2, then, by Lemma A.3, $C_n(i) = \min_j C_n(j)$, and since $\mathbf{E} C_n(U_n) = 0$ when $U_n \sim \text{unif}\{1, \ldots, n\}$, $C_n(i) \leq 0$ and the inequality is trivial.

We may thus assume $i \le n/2$. Since u(1-u) is increasing on [0, 1/2], we may further assume u = i/n. Then, by (2.25),

$$u(1-u)C_n(i) \le u(1-u)\left(C(u) + \frac{3}{n}\right) \le u(1-u)C(u) + \frac{3}{4n}.$$

As stated in [1], it can easily be checked numerically that $\max_{0 \le u \le 1} u(1-u)C(u) < 0.033$, and thus $u(1-u)C_n(i) < 0.05$ follows for $n \ge 45$. The cases $1 \le i \le n \le 44$ are verified numerically. (The maximum value is $591/12005 \doteq 0.0492$, obtained for n = 7 and i = 1 or 7.)

Proof of Theorem A.1. Let $U \sim \text{unif}(0,1)$ and, for $n \ge 1, K \ge 0, \lambda \in \mathbf{R}$,

$$U_{n} := [nU] \sim \operatorname{unif}\{1, \dots, n\},$$

$$W_{n} := \left(\frac{U_{n} - 1}{n}\right)^{2} + \left(\frac{n - U_{n}}{n}\right)^{2} - 1 \leq U^{2} + (1 - U)^{2} - 1 = -2U(1 - U),$$

$$f_{n,K}^{*}(\lambda) := \mathbf{E} \exp\left(\lambda C_{n}(U_{n}) + K\lambda^{2}W_{n}\right),$$

$$f_{n,K}(\lambda) := \mathbf{E} \exp\left(\lambda C_{n}(U_{n}) - 2K\lambda^{2}U(1 - U)\right);$$

note that $f_{n,K}^*(\lambda) \leq f_{n,K}(\lambda)$.

Suppose now that we have found positive numbers K and L such that

$$f_{n,K}^*(\lambda) \le 1, \qquad n \ge 1, \quad \lambda \in [0, L].$$
 (A.3)

Then, by induction, for every $n \ge 0$,

$$\mathbf{E} e^{\lambda Y_n} \le e^{K\lambda^2}, \qquad \lambda \in [0, L].$$
(A.4)

Indeed, (A.4) is trivial for n = 0, and if $n \ge 1$ and $\mathbf{E} e^{\lambda Y_m} \le e^{K\lambda^2}$ for $m \le n-1$ and $\lambda \in [0, L]$, then by the recursion (1.4), for $\lambda \in [0, L]$,

$$\mathbf{E} e^{\lambda Y_n} = \frac{1}{n} \sum_{i=1}^n \mathbf{E} \exp\left[\lambda \left\{\frac{i-1}{n} Y_{i-1} + \frac{n-i}{n} Y_{n-i}^* + C_n(i)\right\}\right]$$
$$= \frac{1}{n} \sum_{i=1}^n \exp[\lambda C_n(i)] \left(\mathbf{E} \exp\left[\lambda \frac{i-1}{n} Y_{i-1}\right]\right) \left(\mathbf{E} \exp\left[\lambda \frac{n-i}{n} Y_{n-i}\right]\right)$$
$$\leq \frac{1}{n} \sum_{i=1}^n \exp[\lambda C_n(i)] \exp\left\{K\lambda^2 \left[\left(\frac{i-1}{n}\right)^2 + \left(\frac{n-i}{n}\right)^2\right]\right\}$$
$$= \mathbf{E} \exp\left[\lambda C_n(U_n) + K\lambda^2(W_n + 1)\right]$$
$$= e^{K\lambda^2} f_{n,K}^*(\lambda) \leq e^{K\lambda^2}.$$

Similarly, if $f_{n,K}^*(\lambda) \leq 1$ for every $n \geq 1$ and $\lambda \in [-L, 0]$, then $\mathbf{E} e^{\lambda Y_n} \leq e^{K\lambda^2}$ for every $n \geq 1$ and $\lambda \in [-L, 0]$.

Thus our goal is to show $f_{n,K}^*(\lambda) \leq 1$ for suitable K and λ ; since $f_{n,K}^*(\lambda) \leq f_{n,K}(\lambda)$, it suffices to show $f_{n,K}(\lambda) \leq 1$. We follow the argument in [1], omitting many details which remain the same.

First, a Taylor expansion yields, using Lemma A.5, for $0 \le \lambda \le L$,

$$f_{n,K}(\lambda) \le 1 + \frac{1}{6}\lambda^2 \left(\sigma^2 - 2K + L \sup_{0 \le \lambda \le L} f_{n,K}^{\prime\prime\prime}(\lambda)\right).$$
(A.5)

Moreover,

$$f_{n,K}^{\prime\prime\prime}(\lambda) = \mathbf{E} \left[\left((C_n(U_n) - 4K\lambda U(1-U))^3 - 12KU(1-U) (C_n(U_n) - 4K\lambda U(1-U)) \right) \times \exp \left(\lambda C_n(U_n) - 2K\lambda^2 U(1-U) \right) \right].$$
(A.6)

Using Lemma A.4, it follows as in [1] that

$$L \sup_{0 \le \lambda \le L} f_{n,K}^{\prime\prime\prime}(\lambda) \le L(3K\eta + 3K^2L)e^L.$$

It is readily checked that for K = 1 and L = 0.42, this is less than $1.547 < 2K - \sigma^2$, so (A.5) shows that $f_{n,1}(\lambda) \leq 1$ for $0 \leq \lambda \leq 0.42$. Hence (A.3) and thus (A.4) hold with K = 1 and L = 0.42.

For larger L we use again Lemma A.4 to obtain

$$f_{n,K}(\lambda) \le e^{|\lambda|} \mathbf{E} \, e^{-2K\lambda^2 U(1-U)}.$$

It is shown in [1] that the right-hand side is at most

$$g_K(\lambda) := e^{|\lambda|} \left[1 - \exp(-K\lambda^2/2) \right] / (K\lambda^2/2)$$

and further that $g_K(\lambda) < 1$ if K = 12 and $0.42 \le \lambda \le 2$, or if $K = 2L^{-2}e^L$ and $2 \le \lambda \le L$. It follows that (A.3) and (A.4) hold for any L > 0 and $K = \max(12, 2L^{-2}e^L)$.

For $-L \leq \lambda \leq 0$, a Taylor expansion yields [cf. (A.5)]

$$f_{n,K}(\lambda) \le 1 + \frac{1}{6}\lambda^2 \left(\sigma^2 - 2K + L \sup_{-L < \lambda \le 0} \left(-f_{n,K}'''(\lambda)\right)\right).$$
 (A.7)

Moreover, from (A.6) and Lemmas A.4 and A.7, for $-L \leq \lambda \leq 0$ we have

$$f_{n,K}^{\prime\prime\prime}(\lambda) \ge (-\eta^3 - 12K \cdot 0.05 - 3K^2L)e^{\eta L}$$

Taking K = 0.5 and L = 0.58, we find

$$L \sup_{-L \le \lambda \le 0} \left(-f_{n,K}^{\prime\prime\prime}(\lambda) \right) < 0.576 < 2K - \sigma^2,$$

and thus by (A.7)

$$f_{n,0.5}(\lambda) \le 1, \qquad -0.58 \le \lambda \le 0.$$
 (A.8)

Finally, for $\lambda \leq -0.58$ we take $K = 2\eta/0.58 < 1.34$. Then $|K\lambda| \geq 2\eta$, and thus, using Lemma A.6,

$$\begin{aligned} \lambda C_n(U_n) + K\lambda^2 W_n &\leq \lambda C_n(U_n) + 2\eta |\lambda| W_n \\ &= -|\lambda| \left[C_n(U_n) - 2\eta \left(\left(\frac{U_n - 1}{n} \right)^2 + \left(\frac{n - U_n}{n} \right)^2 - 1 \right) \right] \leq 0. \end{aligned}$$

Hence $f_{n,K}^*(-\lambda) \leq 1$. (This time we thus use $f_{n,K}^*$ instead of $f_{n,K}$.) Combined with (A.8), this shows that $f_{n,1.34}^*(\lambda) \leq 1$ for all $\lambda \leq 0$, which completes the proof. \Box

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