

A Detailed Analysis of Quicksort Algorithms with Experimental Mathematics

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Abstract

We study several variants of single-pivot and multi-pivot Quicksort algorithms and consider them as discrete probability problems. With experimental mathematics, explicit expressions for expectations, variances and even higher moments of their numbers of comparisons and swaps can be obtained. For some variants, Monte Carlo experiments are performed, the numeric results are demonstrated and the scaled limiting distribution is also discussed.

1 Introduction

A sorting algorithm is an algorithm that rearranges elements of a list in a certain order, the most frequently used orders being numerical order and lexicographical order. Sorting algorithms play a significant role in computer science since efficient sorting is important for optimizing the efficiency of other algorithms which require input data to be in sorted lists. In this paper, our focus is *Quicksort*.

Quicksort was developed by British computer scientist Tony Hoare in 1959 and published in 1961. It has been a commonly used algorithm for sorting since then and is still widely used in industry.

The main idea for Quicksort is that we choose a pivot randomly and then compare the other elements with the pivot, smaller elements being placed on the left side of the pivot and larger elements on the right side of the pivot. Then we recursively apply the same operation to the sublists obtained from the partition step. As for the specific implementations, there can be numerous variants, some of which are at least interesting from a theoretical perspective despite its rare use in the real world.

It is well known that the worst-case performance of Quicksort is $O(n^2)$ and the average performance is $O(n \log n)$. However, we are also interested in the explicit closed-form expressions for the moments of Quicksort's performance, in terms of the number of comparisons and/or the number of swaps. In this paper, only lists or arrays containing distinct elements are considered.

The paper is organized as follows. In section 2, we review related work on the number of comparisons of 1-pivot Quicksort, whose methodology is essential for further study. In section 3, the numbers of swaps of several variants of 1-pivot Quicksort are considered. In section 4, we extend our study to multi-pivot Quicksort. In section 5, the technique to obtain more moments and the scaled limiting distribution are discussed. In the last section we discuss some potential improvements for Quicksort, summarize the main results of this paper and make final remarks on the methodology of experimental mathematics.

Accompanying Maple Package

This article is accompanied by Maple packages `QuickSort.txt` and `Findrec.txt` available from the front of this article

<http://sites.math.rutgers.edu/~yao/QuickSort.html> .

`QuickSort.txt` is the main package of this paper and all procedures mentioned in the paper are from this package unless noted otherwise. `Findrec.txt` is mainly used to find a recurrence relation of moments from the empirical data.

2 Related Work

In the masterpiece of Shalosh B. Ekhad and Doron Zeilberger [EZ1], they managed to find the explicit expressions for expectation, variance and higher moments of the number of comparisons of 1-pivot Quicksort with an experimental mathematics approach, which is also considered as some form of “machine learning”. Here we will review the results they discover or rediscover.

Let C_n be the random variable “number of comparisons in Quicksort applied to lists of length n ”, $n \geq 0$.

Theorem 2.1 ([KP], p.8, end of section 1.3; [GKP], Eq. (2.14), p. 29, and other places)

$$E[C_n] = 2(n+1)H_n - 4n.$$

Here H_n are the *Harmonic numbers*

$$H_n := \sum_{i=1}^n \frac{1}{i}.$$

In following theorems, we introduce the notation

$$H_k(n) := \sum_{i=1}^n \frac{1}{i^k}.$$

Theorem 2.2 (Knuth, [K], answer to Ex. 8(b) in section 6.2.2))

$$\text{var}[C_n] = n(7n+13) - 2(n+1)H_1(n) - 4(n+1)^2H_2(n).$$

Its asymptotic expression is

$$\left(7 - \frac{2}{3}\pi^2\right)n^2 + (13 - 2\ln(n) - 2\gamma - 4/3\pi^2)n - 2\ln(n) - 2\gamma - 2/3\pi^2 + o(1).$$

Theorem 2.3 The third moment about the mean of C_n is

$$-n(19n^2+81n+104)+H_1(n)(14n+14)+12(n+1)^2H_2(n)+16(n+1)^3H_3(n).$$

It is asymptotic to

$$(-19+16\zeta(3))n^3+(-81+2\pi^2+48\zeta(3))n^2+(-104+14\ln(n)+14\gamma+4\pi^2+48\zeta(3))n \\ +14\ln(n)+14\gamma+2\pi^2+16\zeta(3)+o(1).$$

It follows that the limit of the scaled third moment (skewness) converges to

$$\frac{-19+16\zeta(3)}{(7-2/3\pi^2)^{3/2}} = 0.8548818671325885\dots$$

Theorem 2.4 The fourth moment about the mean of C_n is

$$\frac{1}{9}n(2260n^3+9658n^2+15497n+11357)-2(n+1)(42n^2+78n+77)H_1(n) \\ +12(n+1)^2(H_1(n))^2+(-4(42n^2+78n+31)(n+1)^2+48(n+1)^3H_1(n))H_2(n) \\ +48(n+1)^4(H_2(n))^2-96(n+1)^3H_3(n)-96(n+1)^4H_4(n).$$

It is asymptotic to

$$\left(\frac{2260}{9}-28\pi^2+\frac{4}{15}\pi^4\right)n^4+\left(\frac{9658}{9}-84\ln(n)-84\gamma+1/6(-648+48\ln(n)+48\gamma)\pi^2+\frac{16}{15}\pi^4-96\zeta(3)\right)n^3 \\ +\left(\frac{15497}{9}-240\ln(n)-240\gamma+12(\ln(n)+\gamma)^2+1/6(-916+144\ln(n)+144\gamma)\pi^2+8/5\pi^4-288\zeta(3)\right)n^2 \\ +\left(\frac{11357}{9}-310\ln(n)-310\gamma+24(\ln(n)+\gamma)^2+1/6(-560+144\ln(n)+144\gamma)\pi^2+\frac{16}{15}\pi^4-288\zeta(3)\right)n \\ -154\ln(n)-154\gamma+12(\ln(n)+\gamma)^2+1/6(-124+48\ln(n)+48\gamma)\pi^2+\frac{4}{15}\pi^4-96\zeta(3)+o(1).$$

It follows that the limit of the scaled fourth moment (kurtosis) converges to

$$\frac{\frac{2260}{9}-28\pi^2+\frac{4}{15}\pi^4}{(7-2/3\pi^2)^2} = 4.1781156382698542\dots$$

Results for higher moments, more precisely, up to the eighth moment are also discovered and discussed by Shalosh B. Ekhad and Doron Zeilberger in [EZ1].

Before this article, there are already human approaches to find the expectation and variance for the number of comparisons. Let $c_n = E[C_n]$, then since

the pivot can be the k -th smallest element in the list ($k = 1, 2, \dots, n$), we have the recurrence relation

$$c_n = \frac{1}{n} \sum_{k=1}^n ((n-1) + c_{k-1} + c_{n-k}) = (n-1) + \frac{1}{n} \sum_{k=1}^n (c_{k-1} + c_{n-k}) = (n-1) + \frac{2}{n} \sum_{k=1}^n c_{k-1},$$

because the expected number of comparisons for the sublist before the pivot is c_{k-1} and that for the sublist after the pivot is c_{n-k} . From this recurrence relation, the complicated human-generated manipulatorics is needed to rigorously derive the closed form. For the variance, the calculation is much more complicated. For higher moments, we doubt that human approach is realistic.

The experimental mathematics approach is more straightforward and more powerful. For the expectation, a list of data can be obtained through the recurrence relation and the initial condition. Then with an educated guess that c_n is a polynomial of degree one in both n and H_n , i.e.,

$$c_n = a + bn + cH_n + dnH_n$$

where a, b, c, d are undetermined coefficients, we can solve for these coefficients by plugging sufficiently many n and c_n in this equation.

For higher moments, there is a similar recurrence relation for the probability generating function of C_n . With the probability generating function, a list of data of any fixed moment can be obtained. Then with another appropriate educated guess of the form of the higher moments, the explicit expression follows.

In [EZ1], it is already discussed that this experimental mathematics approach is actually rigorous by pointing out that this is a finite calculation and by referring to results in [S1] and [S2].

3 Number of Swaps of 1-Pivot Quicksort

The performance of Quicksort depends on the number of swaps and comparisons performed. In reality, a swap usually takes more computing resources than a comparison. The difficulty to study the number of swaps is that

the number of swaps depends on how to implement the Quicksort algorithm while the number of comparisons are the same despite the specific implementations.

Since only the number of comparisons is considered in [EZ1], the Quicksort model in [EZ1] is that one picks the pivot randomly, compares each non-pivot element with the pivot and then places them in one of the two new lists L_1 and L_2 where the former contains all elements smaller than the pivot and the latter contains those greater than the pivot. Under this model there is no swap, but a lot of memories are needed. For convenience, let's call this model Variant Nulla.

In this section, we consider the random variable, the number of swaps X_n , in different Quicksort variants. Some of them may not be efficient or widely used in industry, however, we treat them as an interesting problem and model in permutation and discrete mathematics. Especially, in the first subsection, we also demonstrate our experimental mathematics approaches step by step.

3.1 Variant I

The first variant is that we always choose the first (or equivalently, the last) element in the list of length n as the pivot, then we compare the other elements with the pivot. We compare the second element with the pivot first. If it is greater than the pivot, it stays where it is, otherwise we put it before the pivot and all the other elements including the pivot shift one position to the right. Though this is somewhat different from the “traditional swap”, we define this operation as a swap. Generally, every time we find an element smaller than the pivot, we put it on the pivot's current position and the indexes of the pivot and all elements on the right of pivot plus one.

Hence, after $n - 1$ comparisons and some number of swaps, the partition is achieved, i.e., all elements on the left of the pivot is smaller than the pivot and all elements on the right of the pivot is greater than the pivot. The difference between this variant and Variant Nulla is that this one does not need to create new lists so that it saves memories.

Let $P_n(t)$ be the probability generating function for the number of swaps,

i.e.,

$$P_n(t) = \sum_{k=0}^{\infty} P(X_n = k) t^k,$$

where for only finitely many integers k , $P(X_n = k)$ is nonzero.

We have the recurrence relation

$$P_n(t) = \frac{1}{n} \sum_{k=1}^n P_{k-1}(t) P_{n-k}(t) t^{k-1},$$

with the initial condition $P_0(t) = P_1(t) = 1$ because for any fixed $k \in \{1, 2, \dots, n\}$, the probability that the pivot is the k -th smallest is $\frac{1}{n}$ and there are exactly $k - 1$ swaps when the pivot is the k -th smallest.

The Maple procedure `SwapPqs(n,t)` in the package `Quicksort.txt`, which is the accompanying Maple package of the paper, implements the recurrence of the probability generating function.

Recall that the r -th moment is given in terms of the probability generating function

$$E[X_n^r] = \left(t \frac{d}{dt}\right)^r P_n(t) \Big|_{t=1}.$$

The moment about the mean

$$m_r(n) := E[(X_n - c_n)^r],$$

can be easily derived from the raw moments $\{E[X_n^l] \mid 1 \leq l \leq r\}$, using the binomial theorem and linearity of expectation. Another way to get the moment about the mean is by considering

$$m_r(n) = \left(t \frac{d}{dt}\right)^r \left(\frac{P_n(t)}{t^{c_n}}\right) \Big|_{t=1}.$$

Recall that

$$H_k(n) := \sum_{i=1}^n \frac{1}{i^k}.$$

Our educated guess is that there exists a polynomial of $r + 1$ variables $F_r(x_0, x_1, \dots, x_n)$ such that

$$m_r(n) = F_r(n, H_1(n), \dots, H_r(n)).$$

With the Maple procedure `QsMFn`, we can easily obtain the following theorems by just entering `QsMFn(SwapPQs, t, n, Hn, r)` where r represents the moment you are interested in. When $r = 1$, it returns the explicit expression for its mean rather than the trivial “first moment about the mean”.

Theorem 3.1.1 The expectation of the number of swaps of Quicksort for a list of length n under Variant I

$$E[X_n] = (n + 1)H_n - 2n.$$

Theorem 3.1.2 The variance of X_n is

$$2n(n + 2) - (n + 1)H_1(n) - (n + 1)^2H_2(n).$$

Theorem 3.1.3 The third moment about the mean of X_n is

$$-\frac{9}{4}n(n + 3)^2 + (4n + 4)H_1(n) + 3(n + 1)^2H_2(n) + 2(n + 1)^3H_3(n).$$

Theorem 3.1.4 The fourth moment about the mean of X_n is

$$\begin{aligned} & \frac{1}{18}n(335n^3 + 1568n^2 + 3067n + 2770) - 3(n + 1)(4n^2 + 8n + 9)H_1(n) + 3(n + 1)^2H_1(n)^2 \\ & - (12n^2 + 24n + 19)(n + 1)^2 + 6(n + 1)^3H_1(n)H_2(n) + 3(n + 1)^4H_2(n)^2 \\ & - 12(n + 1)^3H_3(n) - 6(n + 1)^4H_4(n). \end{aligned}$$

The explicit expressions for higher moments can be easily calculated automatically with the Maple procedure `QsMFn` and the interested readers are encouraged to find those formulas on their own.

3.2 Variant II

The second variant is similar with the first one. One tiny difference is that instead of choosing the first or last element as the pivot, the index of the pivot is chosen uniformly at random. For example, we choose the i -th element, which is the k -th smallest, as the pivot. Then we compare those non-pivot elements with the pivot. If $i \neq 1$, the first element will be compared with

the pivot first. If it is smaller than the pivot, it stays there, otherwise it is moved to the end of the list and all other elements including the pivot shift one position to the left. After comparing all the left-side elements with the pivot, we look at those elements whose indexes are originally greater than i . If they are greater than the pivot, no swap, otherwise move them to the pivot's current position and the indexes of the pivot and elements after the pivot but before the swapped element now plus one.

In this case, the recurrence of the probability generating function $P_n(t)$ is more complicated as a consequence of that the number of swaps given that i and k is known is still a random variable rather than a fixed number as the case in Variant I.

Let $Q(n, k, i, t)$ be the probability generating function for such a random variable. In fact, given a random permutation in the permutation group S_n and that the i -th element is k , the number of swaps equals to the number of elements which are before k and greater than k or after k and smaller than k . Hence, if there are j elements which are before k and smaller than k , then there are $i - 1 - j$ elements which are before k and greater than k and there are $k - 1 - j$ elements which are after k and smaller than k . So in this case the number of swaps is $i + k - 2 - 2j$.

Then we need to determine the range of j . Obviously it is at least 0. Totally there are $k - 1$ elements which are less than k , at most $n - i$ of them is after k , so $j \geq k - 1 - n + i$. As for the upper bound, since there are only $i - 1$ elements before k , $j \leq i - 1$. Evidently, $j \leq k - 1$ as well. Therefore the range of j is $[\max(k - 1 - n + i, 0), \min(i - 1, k - 1)]$.

As for the probability that there are exactly j elements which are before k and smaller than k , it equals to

$$\binom{i-1}{j} \prod_{s=0}^{j-1} \frac{k-1-s}{n-1-s} \prod_{s=0}^{i-j-2} \frac{n-k-s}{n-1-j-s}.$$

Consequently, the probability generating function

$$Q(n, k, i, t) = \sum_{j=\max(k-1-n+i, 0)}^{\min(i-1, k-1)} \binom{i-1}{j} \prod_{s=0}^{j-1} \frac{k-1-s}{n-1-s} \prod_{s=0}^{i-j-2} \frac{n-k-s}{n-1-j-s} t^{i+k-2-2j},$$

which is implemented by the Maple procedure `PerProb(n, k, i, t)`. For example, `PerProb(9, 5, 5, t)` returns

$$\frac{1}{70}t^8 + \frac{8}{35}t^6 + \frac{18}{35}t^4 + \frac{8}{35}t^2 + \frac{1}{70}.$$

We have the recurrence relation

$$P_n(t) = \frac{1}{n^2} \sum_{k=1}^n \sum_{i=1}^n P_{k-1}(t)P_{n-k}(t)Q(n, k, i, t),$$

with the initial condition $P_0(t) = P_1(t) = 1$, which is implemented by the Maple procedure `SwapPQ(n, t)`. The following theorems follow immediately.

Theorem 3.2.1 The expectation of the number of swaps of Quicksort for a list of length n under Variant II

$$E[X_n] = (n + 1)H_n - 2n.$$

Theorem 3.2.2 The variance of X_n is

$$\frac{1}{6}n(11n + 17) - \frac{1}{3}(n + 1)H_1(n) - (n + 1)^2H_2(n).$$

Theorem 3.2.3 The third moment about the mean of X_n is

$$-\frac{1}{6}n(14n^2 + 57n + 73) + (2n + 2)H_1(n) + (n + 1)^2H_2(n) + 2(n + 1)^3H_3(n).$$

Theorem 3.2.4 The fourth moment about the mean of X_n is

$$\begin{aligned} & \frac{1}{90}n(1496n^3 + 5531n^2 + 8527n + 6922) - \frac{1}{15}(n+1)(55n^2 + 85n + 173)H_1(n) + \frac{1}{3}(n+1)^2H_1(n)^2 \\ & \left(-\frac{1}{3}(33n^2 + 51n + 25)(n + 1)^2 + 2(n + 1)^3H_1(n)\right)H_2(n) + 3(n + 1)^4H_2(n)^2 \\ & - 4(n + 1)^3H_3(n) - 6(n + 1)^4H_4(n). \end{aligned}$$

Higher moments can also be easily obtained by entering `QsMFn(SwapPQ, t, n, Hn, r)` where r represents the r -th moment you are interested in.

Comparing with the Variant I where the index of the pivot is fixed, we find that these two variants have the same expected number of swaps. However, the variance and actually all even moments of the second variant are smaller. Considering that the average performance is already $O(n \log n)$ which is not far from the best scenario, it is favorable that a Quicksort algorithm has smaller variance. In conclusion, for this model, a randomly-chosen-index pivot can improve the performance of the algorithm.

3.3 Variant III

Next we'd like to study the most widely used in-place Quicksort. This algorithm is called Lomuto partition scheme, which is attributed to Nico Lomuto and popularized by Bentley in his book *Programming Pearls* and Cormen, *et al.* in their book *Introduction to Algorithms*. This scheme chooses a pivot that is typically the last element in the list. Two indexes, i , the insertion index, and j , the search index are maintained. Following is the pseudo code for this variant.

algorithm quicksort(A , s , t) is

```

if  $s < t$  then
     $p := \text{partition}(A, s, t)$ 
    quicksort( $A, s, p - 1$ )
    quicksort( $A, p + 1, t$ )

```

algorithm partition(A , s , t) is

```

pivot :=  $A[t]$ 
 $i := s$ 
for  $j := s$  to  $t - 1$  do
    if  $A[j] < \text{pivot}$  then
        swap  $A[i]$  with  $A[j]$ 
         $i := i + 1$ 
swap  $A[i]$  with  $A[t]$ 

```

return `i`

From the algorithm we can see that when the pivot is the k -th smallest, there are $k - 1$ elements smaller than the pivot. As a result, there are $k - 1$ swaps in the `if` statement of the algorithm `partition`. Including the last swap outside the `if` statement, there are totally k swaps. We have the recurrence relation for its probability generating function

$$P_n(t) = \frac{1}{n} \sum_{k=1}^n P_{k-1}(t) P_{n-k}(t) t^k$$

with the initial condition $P_0(t) = P_1(t) = 1$.

Theorem 3.3.1 The expectation of the number of swaps of Quicksort for a list of length n under Variant III

$$E[X_n] = (n + 1)H_n - \frac{4}{3}n - \frac{1}{3}.$$

Theorem 3.3.2 The variance of the number of swaps of Quicksort for a list of length n under Variant III

$$\text{var}[X_n] = 2n^2 + \frac{187}{45}n + \frac{7}{45} - \frac{2}{3n} - (n^2 + 2n + 1)H_2(n) - (n + 1)H_1(n).$$

Note that for this variant, and some other ones in the remainder of the paper, to find out its explicit expression of moments, we may need to modify our educated guess to a “rational function” of n and $H_k(n)$ for some k (see procedure `QsMFnRat` and `QsMFnRatG`). Moreover, sometimes when we solve the equations obtained by equalizing the guess with the empirical data, some initial terms should be disregarded since the increasing complexity of the definition of the Quicksort algorithms may lead to the “singularity” of the first several terms of moments. Usually, the higher the moment is, the more initial terms should be disregarded.

3.4 Variant IV

In Variant III, every time when `A[j] < pivot`, we swap `A[i]` with `A[j]`. However, it is a waste to swap them when $i = j$. If we modify the algorithm

such that a swap is performed only when the indexes $i \neq j$, the expected cost will be reduced. Besides, if the pivot is actually the largest element, there is no need to swap $A[i]$ with $A[t]$ in the partition algorithm. To popularize Maple in mathematical and scientific research, we attach Maple code for the partition part here, the `ParIP` procedure in the package `QuickSort.txt`, in which `Swap(S, i, j)` is a subroutine to swap the i -th element with the j -th in a list S .

```

ParIP:=proc(L) local pivot,i,j,n,S:
n:=nops(L):
pivot:=L[n]:
S:=L:
i:=1:
for j from 1 to n-1 do
  if S[j]<=pivot then
    if i<>j then
      S:=Swap(S, i, j):
      i:=i+1:
    else
      i:=i+1:
    fi:
  fi:
od:
if i<>n then
  return Swap(S, i, n), i:
else
  return S, i:
fi:

```

end:

Lemma 3.4.1 Let $Y_n(k)$ be the number of swaps needed in the first partition step in an in-place Quicksort without swapping the same index for a list L of length n when the pivot is the k -th smallest element, then

$$Y_n(k) = \begin{cases} |\{i \in [n] \mid L[i] \leq \text{pivot}; \exists j < i, L[j] > \text{pivot}\}| & k < n \\ 0 & k = n \end{cases}.$$

Proof. When $k = n$, it is obviously that for each search index j , the condition $S[j] \leq \text{pivot}$ is satisfied, hence the insertion index i is always equal to j , which means there is no swap inside the loop. Since eventually $i = n$, there is also no need to swap the pivot with itself. So the number of swaps is 0 in this case.

When $k < n$, notice that the first time i is smaller than j is when we find the first element greater than the pivot. After that, i will be always less than j , which implies that for each element smaller than the pivot and the pivot itself, one swap is performed. \square

The Maple procedure `IPProb(n, k, t)` takes inputs n, k as defined above and a symbol t , output the probability generating function $Q(n, k, t)$ for the number of swaps in the first partition when the length of the list is n and the last element, which is chosen as the pivot, is the k -th smallest.

When $k < n$, the probability that there are s swaps is

$$\binom{k-1}{k-s} \frac{(k-s)!(n-k)(n-k-2+s)!}{(n-1)!}.$$

Therefore the probability generating function

$$Q(n, k, t) = \sum_{s=1}^k \binom{k-1}{k-s} \frac{(k-s)!(n-k)(n-k-2+s)!}{(n-1)!} t^s.$$

The recurrence relation for the probability generating function $P_n(t)$ of the total number of swaps follows immediately

$$P_n(t) = \frac{1}{n} \sum_{k=1}^n P_{k-1}(t) P_{n-k}(t) Q(n, k, t)$$

with the initial condition $P_0(t) = P_1(t) = 1$.

Theorem 3.4.2 The expectation of the number of swaps of Quicksort for a list of length n under Variant IV

$$E[X_n] = (n + 2)H_n - \frac{5}{2}n - \frac{1}{2}.$$

Theorem 3.4.3 The variance of the number of swaps of Quicksort for a list of length n under Variant IV

$$\text{var}[X_n] = 2n^2 - \frac{215}{12}n + \frac{1}{12} + (11n+14)H_1(n) - (n^2-2n-2)H_2(n) - (2n+2)H_1(n)^2$$

Compare these results with **Theorem 3.1.1** and **Theorem 3.2.1**, it shows that Variant IV has better average performances, notwithstanding the “broader” definition of “swap” in the first two subsections. And of course, it is better than the in-place Quicksort which swaps the indexes even when they are the same. We fully believe that the additional cost to check whether the insertion and search indexes are the same are totally worth.

3.5 Variant V

This variant might not be practical, but we find that it is interesting as a combinatorial model. As is well known, if a middle-most element is chosen as a pivot, the Quicksort algorithm will have better performance than average in this case. Hence if additional information is available so that the probability distribution of chosen pivots is no longer a uniform distribution but something like a bell curve, it is to our advantage.

Assume that the list is a permutation of $[n]$ and we are trying to sort it, pretending that we do not know the sorted list must be $[1, 2, \dots, n]$. Now the rule is that we choose the first and last number in the list, look at the numbers and choose the one which is closer to the middle. If the two numbers are equally close to the middle, then flip a coin to decide the final choice.

Without loss of generality, we can always assume that the last element in the list is chosen as the pivot, otherwise we just need to run the algorithm in the last subsection “reversely”, putting both the insertion and search indexes

on the last element and letting larger elements be swapped to the left side of the pivot, etc. So the only difference with Variant IV is the probability distribution of k , which is no longer $\frac{1}{n}$ for each $k \in [n]$.

By symmetry, $Pr^{(n)}(\text{pivot} = k) = Pr^{(n)}(\text{pivot} = n + 1 - k)$, so we only need to consider $1 \leq k \leq (n + 1)/2$. When n is even, let $n = 2m$. Then $Pr^{(n)}(\text{pivot} = k) = \frac{4k-3}{(2m-1)2m}$. When n is odd, let $n = 2m - 1$, then $Pr^{(n)}(\text{pivot} = k) = \frac{4k-3}{(2m-1)(2m-2)}$ when $k < m$ and $Pr^{(n)}(\text{pivot} = m) = \frac{2}{2m-1}$.

With this minor modification, the recurrence relation for $P_n(t)$ follows.

$$P_n(t) = \sum_{k=1}^n P_{k-1}(t)P_{n-k}(t)Q(n, k, t)Pr^{(n)}(\text{pivot} = k)$$

with the initial condition $P_0(t) = P_1(t) = 1$.

Though an explicit expression seems difficult in this case, we can still analyze the performance of the algorithm by evaluating its expected number of swaps. By exploiting the Maple procedure `MomFn(f, t, m, N)`, which inputs a function name f , a symbol t , the order of the moment m and the upper bound of the length of the list N and outputs a list of m -th moments for the Quicksort described by the probability generating function f of lists of length $1, 2, \dots, N$, we find that Variant V has better average performance than Variant IV when n is large enough. For example, `MomFn(PQIP, t, 1, 20)` returns

$$\left[0, \frac{1}{2}, \frac{7}{6}, 2, \frac{179}{60}, \frac{41}{10}, \frac{747}{140}, \frac{187}{28}, \frac{20459}{2520}, \frac{1013}{105}, \frac{312083}{27720}, \frac{25631}{1980}, \frac{353201}{24024}, \frac{1488737}{90090}, \frac{6634189}{360360}, \frac{814939}{40040}, \frac{273855917}{12252240}, \frac{4983019}{204204}, \frac{97930039}{3695120}, \frac{20210819}{705432}\right],$$

and `MomFn(PQIPk, t, 1, 20)` returns

$$\left[0, \frac{1}{2}, \frac{4}{3}, \frac{20}{9}, \frac{155}{48}, \frac{1957}{450}, \frac{2341}{420}, \frac{4055}{588}, \frac{55829}{6720}, \frac{794}{81}, \frac{630547}{55440}, \frac{170095}{13068}, \frac{12735487}{864864}, \frac{3864281}{234234}, \frac{2521865}{137592}, \frac{36424327}{1801800}, \frac{4343228489}{196035840}, \frac{107768347}{4463316}, \frac{15673532207}{598609440}, \frac{1136599735}{40209624}\right].$$

We notice that since $n \geq 14$, Variant V consistently has better average performance. From this result we can conclude that it is worth choosing a

pivot from two candidates since the gains of efficiency are way more than its cost.

Moreover, we can obtain a recurrence for the expected number x_n of the random variable X_n . The `Findrec(f,n,N,MaxC)` procedure in the Maple package `Findrec.txt` inputs a list of data L , two symbols n and N , where n is the discrete variable, and N is the shift operator, and $MaxC$ which is the maximum degree plus order. `Findrec(MomFn(PQIPk, t, 1, 80), n, N, 11)` returns

$$\begin{aligned} & \frac{n(n-1)(n+1)(124300966127n^2 + 675726017124n + 650712665709)}{(n+7)(n+6)(n+5)(17482518431n^2 + 498259584530n + 1781699167235)} - \frac{2n(n+2)(n+1)(216417203729n^2 + 919675870477n + 92300503754)N}{(n+7)(n+6)(n+5)(17482518431n^2 + 498259584530n + 1781699167235)} \\ & + \frac{(n+2)(n+1)(350982431977n^3 + 911174904749n^2 - 6154705279825n - 16672650937797)N^2}{(n+7)(n+6)(n+5)(17482518431n^2 + 498259584530n + 1781699167235)} \\ & + \frac{4(n+2)(70891742279n^4 + 1238063051796n^3 + 6234404912517n^2 + 8329928119664n - 5599544780136)N^3}{(n+7)(n+6)(n+5)(17482518431n^2 + 498259584530n + 1781699167235)} \\ & - \frac{(n+3)(492765916535n^4 + 5467106459287n^3 + 8863038802013n^2 - 71364745940767n - 204534459680620)N^4}{(n+7)(n+6)(n+5)(17482518431n^2 + 498259584530n + 1781699167235)} \\ & + \frac{2(n+4)(74633719171n^5 - 190797245354n^4 - 6602055805627n - 18802118680054)N^5}{(n+7)(n+5)(17482518431n^2 + 498259584530n + 1781699167235)} + N^6 \end{aligned}$$

Figure 1: The Recurrence Relation for the Expected Number of Swaps

As aforementioned, N is a shift operator. Since this formula is too long, to see its detailed interpretation, please look at **Theorem 4.2.1** as reference.

For sure we can also look at more elements to choose the middle-most one as the pivot. In case that we do not want to store so much information, some other variants involving “look twice” idea could be that if the first selected element is within some satisfactory interval, e.g., $[\frac{n}{4}, \frac{3n}{4}]$ for a permutation of n , then it is chosen as the pivot. Otherwise we choose a second element as the pivot without storing information about the first one. It is also likely to improve the algorithm with “multiple looks” to choose the pivot and the requirement to choose the current element as the pivot without continuing looking at the next one could vary and ideally the requirement should be more relaxed as the number of “looks” goes up.

4 Explorations for Multi-Pivot Quicksort

With the same general idea of the 1-pivot Quicksort, it is natural to think about “what if we choose more pivots”. In k -pivot Quicksort, k indexes are

chosen and the correspondent elements become pivots. The k pivots need to be sorted and then the other elements will be partitioned into one of the $k + 1$ sublists. Compared to 1-pivot Quicksort, multi-pivot Quicksort is much more complicated because we need to determine how to sort the pivots, how to allocate each non-pivot element to the sublist they belong to and how to sort a sublist containing less than k elements. Therefore, there are a few multi-pivot Quicksort variants. We refer the readers to [I2] for other versions of multi-pivot. When k is large, it seems difficult to have an in-place version, so we mainly consider the random variable, the number of comparisons C_n , in this section since a swap might be difficult to define in this case.

4.1 Dual-Pivot Quicksort

Let's start from the simplest multi-pivot Quicksort: dual-pivot. The model for dual-pivot Quicksort is that two pivots p_1 and p_2 are randomly chosen. After one comparison, they are sorted, say $p_1 < p_2$. Non-pivot elements should be partitioned into one of the three sublists L_1, L_2 and L_3 . L_1 contains elements smaller than p_1 , L_2 contains elements between p_1 and p_2 while L_3 contains elements greater than p_2 . Each non-pivot element is compared with p_1 first. If it is smaller than p_1 , we are done. Otherwise it is compared with p_2 to determine whether it should go to L_2 or L_3 .

Given that the list contains n distinct elements and the two pivots are the i -th and j -th smallest element ($i < j$), we need one comparison to sort the pivot and $i - 1 + 2(n - i - 1) = 2n - i - 3$ comparisons to distribute non-pivot elements to the sublists. Hence the total number is $2n - i - 2$ and the recurrence relation for the probability generating function $P_n(t)$ of the total number of comparisons C_n of dual-pivot Quicksort is

$$P_n(t) = \frac{1}{\binom{n}{2}} \sum_{j=2}^n \sum_{i=1}^{j-1} P_{i-1}(t) P_{j-i-1}(t) P_{n-j}(t) t^{2n-i-2}$$

with the initial condition $P_0(t) = P_1(t) = 1$ and $P_2(t) = t$.

The above recurrence is implemented by the procedure `PQc2`. With the aforementioned Maple procedure `QsMFn` it is easy to get the following theorems.

Theorem 4.1.1 The expectation of the number of comparisons in dual-pivot Quicksort algorithms

$$E[C_n] = 2(n+1)H_n - 4n.$$

Theorem 4.1.2 The variance of the number of comparisons in dual-pivot Quicksort algorithms

$$\text{var}[C_n] = n(7n+13) - 2(n+1)H_1(n) - 4(n+1)^2H_2(n).$$

Theorem 4.1.3 The third moment about the mean of C_n is

$$-n(19n^2+81n+104)+H_1(n)(14n+14)+12(n+1)^2H_2(n)+16(n+1)^3H_3(n).$$

Theorem 4.1.4 The fourth moment about the mean of C_n is

$$\begin{aligned} & \frac{1}{9}n(2260n^3+9658n^2+15497n+11357) - 2(n+1)(42n^2+78n+77)H_1(n) \\ & +12(n+1)^2(H_1(n))^2 + (-4(42n^2+78n+31)(n+1)^2+48(n+1)^3H_1(n))H_2(n) \\ & +48(n+1)^4(H_2(n))^2 - 96(n+1)^3H_3(n) - 96(n+1)^4H_4(n). \end{aligned}$$

As usual, any higher moment could be easily obtained with a powerful silicon servant. Careful readers may notice that the above four theorems are exactly the same with the ones in section 2. It is natural to ask whether they have indeed the same probability distribution. The answer is yes. In section 4.1.2 of [I1] the author gives a sketch of proof showing that actually 1-pivot and dual-pivot Quicksort's numbers of comparisons satisfy the same recurrence relation and initial condition. From experimental mathematical point of view, a semi-rigorous proof obtained by checking sufficiently many special cases is good enough for us. For example, the first 10 probability generating function, $P_n(t)$ for $1 \leq n \leq 10$ can be calculated in a nanosecond by entering [seq(PQc2(i, t), i = 1..10)] and we have

$$P_1(t) = 1,$$

$$P_2(t) = t,$$

$$P_3(t) = \frac{2}{3}t^3 + \frac{1}{3}t^2,$$

$$\begin{aligned}
P_4(t) &= \frac{1}{3}t^6 + \frac{1}{6}t^5 + \frac{1}{2}t^4, \\
P_5(t) &= \frac{2}{15}t^{10} + \frac{1}{15}t^9 + \frac{1}{5}t^8 + \frac{4}{15}t^7 + \frac{1}{3}t^6, \\
&\dots \quad \dots \quad \dots
\end{aligned}$$

which are exactly the same with the probability generating function for the number of comparisons of 1-pivot Quicksort.

In conclusion, in terms of probability distribution of the number of comparisons, the dual-pivot Quicksort does not appear to be better than the ordinary 1-pivot Quicksort.

As for the random variable X_n , the number of swaps, it depends on the specific implementation of the algorithm and the definition of a “swap”. As a toy model, we do an analogue of section 3.1. Assume the list is a permutation of $[n]$. The first and last elements are chosen as the pivot. Let’s say they are i and j . If $i > j$ then we swap them and still call the smaller pivot i . For each element less than i , we move it to the left of i , and for each element greater than j , we move it to the right of j and call this kind of operations a swap.

The recurrence relation for the probability generating function of X_n is

$$P_n(t) = \frac{1}{\binom{n}{2}} \left(\frac{1}{2} + \frac{1}{2}t \right) \sum_{j=2}^n \sum_{i=1}^{j-1} P_{i-1}(t) P_{j-i-1}(t) P_{n-j}(t) t^{n-1+i-j}$$

with the initial conditions $P_0(t) = P_1(t) = 1$ and $P_2(t) = \frac{1}{2} + \frac{1}{2}t$.

Theorem 4.1.5 The expectation of the number of swaps in the above dual-pivot Quicksort variant

$$E[X_n] = \frac{4}{5}(n+1)H_n - \frac{39}{25}n - \frac{1}{100}.$$

Note that this result is better than those in section 3.1 and 3.2.

4.2 Three-Pivot Quicksort

As mentioned at the beginning of this section, to define a 3-pivot Quicksort, we need to define 1) how to sort the pivots, 2) how to partition the list and

3) how to sort a list or sublist containing less than 3 pivots. Since this paper is to study Quicksort, we choose 1-pivot Quicksort for 1) and 3). For 2), it seems that the binary search is a good option since for each non-pivot element exactly 2 comparisons with the pivots are needed.

The Maple procedure `PQs(n, t)` outputs the probability generating function for 1-pivot Quicksort of a list of length n . Hence during the process of sorting the pivots and partitioning the list, the probability generating function of the number of comparisons is $PQs(3, t)t^{2n-6}$, which equals to

$$\left(\frac{2}{3}t^3 + \frac{1}{3}t^2\right)t^{2n-6} = \frac{2}{3}t^{2n-3} + \frac{1}{3}t^{2n-4}.$$

So the recurrence relation for the probability generating function $P_n(t)$ of the total number of comparisons for 3-pivot Quicksort of a list of length n is

$$P_n(t) = \frac{1}{\binom{n}{3}} \sum_{k=3}^n \sum_{j=2}^{k-1} \sum_{i=1}^{j-1} P_{i-1}(t)P_{j-i-1}(t)P_{k-j-1}(t)P_{n-k}(t)\left(\frac{2}{3}t^{2n-3} + \frac{1}{3}t^{2n-4}\right)$$

with initial conditions $P_0(t) = P_1(t) = 1$, $P_2(t) = t$ and $P_3(t) = \frac{2}{3}t^3 + \frac{1}{3}t^2$. This recurrence is implemented by the procedure `PQd3`.

The explicit expression seems to be difficult to obtained in this case, but numerical tests imply that 3-pivot Quicksort has better performances than dual-pivot, and of course 1-pivot since it is indeed equivalent to dual-pivot.

By exploiting the Maple procedure `MomFn(f, t, m, N)` again, we can compare the expectation of different Quicksort variants.

For instance, `MomFn(PQc2, t, 1, 20)` returns

$$\left[0, 1, \frac{8}{3}, \frac{29}{6}, \frac{37}{5}, \frac{103}{10}, \frac{472}{35}, \frac{2369}{140}, \frac{2593}{126}, \frac{30791}{1260}, \frac{32891}{1155}, \frac{452993}{13860}, \frac{476753}{12870}, \frac{499061}{12012}, \frac{2080328}{45045}, \frac{18358463}{360360}, \frac{18999103}{340340}, \frac{124184839}{2042040}, \frac{127860511}{1939938}, \frac{26274175}{369512}\right],$$

and `MomFn(PQd3, t, 1, 20)` returns

$$\left[0, 1, \frac{8}{3}, \frac{14}{3}, \frac{106}{15}, \frac{49}{5}, \frac{64}{5}, \frac{561}{35}, \frac{1226}{63}, \frac{5192}{225}, \frac{465316}{17325}, \frac{533509}{17325}, \frac{714008}{20475}, \frac{61615768}{1576575}, \frac{342234824}{7882875}, \frac{754600981}{15765750}, \frac{1404956027}{26801775}, \frac{15298397599}{268017750}, \frac{31489234438}{509233725}, \frac{1697926310039}{25461686250}\right].$$

We notice that for each fixed $n > 3$, 3-pivot Quicksort's average performance is better than 2-pivot and 1-pivot. This numerical test is also doable for all previous Quicksort variants but seems unnecessary when the explicit expressions are easily accessible.

Similarly with section 3.5, a recurrence relation of the expected number of comparisons can be obtained. `Findrec(MomFn(PQd3, t, 1, 40), n, N, 8)` returns

$$\begin{aligned} & \frac{(3n+4)(n^2-5n+12)}{(n+4)(n+3)(3n+1)} - \frac{(12n^4+13n^3-12n^2+59n+24)N}{(3n+1)(n+4)(n+3)(n+2)} \\ & + 3 \frac{(n+1)(6n+5)nN^2}{(n+4)(n+3)(3n+1)} - \frac{(n+1)(12n+7)N^3}{(n+4)(3n+1)} + N^4, \end{aligned}$$

which leads to the following theorem.

Theorem 4.2.1 The expected number of comparisons C_n of 3-pivot Quicksort for a list of length n satisfies the following recurrence relation

$$\begin{aligned} C_{n+4} &= \frac{(n+1)(12n+7)}{(n+4)(3n+1)}C_{n+3} - 3 \frac{(n+1)(6n+5)n}{(n+4)(n+3)(3n+1)}C_{n+2} \\ &+ \frac{(12n^4+13n^3-12n^2+59n+24)}{(3n+1)(n+4)(n+3)(n+2)}C_{n+1} - \frac{(3n+4)(n^2-5n+12)}{(n+4)(n+3)(3n+1)}C_n. \end{aligned}$$

The recurrence relations for higher moments are also obtainable, but a long enough list of data is needed.

4.3 k -Pivot Quicksort

More generally, k -pivot Quicksort can be considered with the convention that 1) the k pivots are sorted with 1-pivot Quicksort, 2) binary search is used to partition the list into $k+1$ sublists, 3) we use 1-pivot Quicksort to sort lists with length less than k .

In the package `QuickSort.txt` the procedure `PQck(n, t, k)` outputs the probability generating function for the number of comparisons of k -pivot Quicksort where each element is compared with pivots in a linearly increasing order. Obviously this is not efficient when k is large. However, the problem for binary search is that when $k \neq 2^i - 1$ for some i , it is hard to

get an expression for the number of comparisons in the binary search step since the number highly depends on the specific implementation where some boundary cases may vary and the floor and ceiling functions will be involved, which leads to an increasing difficulty to find the explicit expressions for moments.

There is a procedure $\text{QsBC}(L, k)$ which inputs a list of distinct numbers L and an integer k representing the number of pivots and outputs the sorted list and the total number of comparisons. For convenience of Monte Carlo experiments, we use $\text{MCQsBC}(n, k, T)$ where n is the length of the list, k is the number of pivots and T is the number of times we repeat the experiments. Because of the limit of computing resources, we only test for $k = 3, 4, 5, 6$ and $n = 10, 20, 30, 40, 50$.

$$[\text{seq}(\text{MCQsBC}(10 * i, 3, 100), i = 1..5)] = [22.95, 65.75, 118.71, 178.28, 239.45],$$

$$[\text{seq}(\text{MCQsBC}(10 * i, 4, 100), i = 1..5)] = [23.78, 67.77, 120.91, 180.35, 251.19],$$

$$[\text{seq}(\text{MCQsBC}(10 * i, 5, 100), i = 1..5)] = [23.54, 65.74, 119.59, 178.36, 241.03],$$

$$[\text{seq}(\text{MCQsBC}(10 * i, 6, 100), i = 1..5)] = [23.14, 66.22, 120.07, 176.43, 236.46],$$

Our observation is that for large enough n , the more pivots we use, the less comparisons are needed. However, when k is too close to n , the increase of pivots may lead to inefficiency.

5 Limiting Distribution

The main purpose of this paper is to find explicit expressions for the moments of the number of swaps or comparisons of some variants of Quicksort, to compare their performances and to explore more efficient Quicksort algorithms.

However, it is also of interest to find more moments for large n and calculate their floating number approximation of the scaled limiting distribution.

As mentioned in [EZ1], if we are only interested in the first few moments, then it is wasteful to compute the full probability generating function $P_n(t)$. Let $t = 1 + w$ and use the fact that

$$P_n(1 + w) = \sum_{r=0}^{\infty} \frac{f_r(n)}{r!} w^r$$

where $f_r(n)$ are the factorial moments. The straight moments $E[X_n^r]$, and the moments-about-the-mean, $m_r(n)$ follow immediately.

As a case study, let's use the Variant IV in section 3.4 as an example. The recurrence relation is

$$P_n(1 + w) = \frac{1}{n} \sum_{k=1}^n P_{k-1}(1 + w) P_{n-k}(1 + w) Q(n, k, 1 + w),$$

where Q is as defined in 3.4.

Since only the first several factorial moments are considered, in each step truncation is performed and only the first several coefficients in w is kept. With this method we can get more moments in a fixed time. The procedure **TrunIP** implements the truncated factorial generating function.

With the closed-form expressions for both the expectation, c_n , and the variance $m_2(n) := \text{var}(X_n)$, the scaled random variable Z_n is defined as follows.

$$Z_n := \frac{X_n - c_n}{\sqrt{m_2(n)}}.$$

We are interested in the floating point approximations of the limiting distribution $\lim_{n \rightarrow \infty} Z_n$. Of course its expectation is 0 and its variance is 1.

For instance, if we'd like to know the moments up to order 10, **TrunIP**(100, z, 10) returns

$$1 + \frac{7617634712836831344646726224164628686543}{27341323619495089084130905464828354336} z + \frac{1169146867836246319480317311960440606057785761234433183813484643}{29517287662514914280390084303910684938635848245569645536000} z^2$$

$$+ \frac{58024172013839694810625346567417182291098218339356411215067112605982034521}{15125688216961909953814450921738787993181911018772132633289881600000} z^3$$

$$+ \dots$$

For $1 \leq r \leq 10$, the coefficient of x^r times $r!$ is the r -th factorial moment. By

$$E[X^r] = \sum_{j=0}^r \left\{ \begin{matrix} r \\ j \end{matrix} \right\} E[(X)_j]$$

where the curly braces denote Stirling numbers of the second kind, we can get the raw moments. And with the procedure `MtoA` a sequence of raw moments are transformed to moments about the mean. Divided by $m_2(n)^{\frac{r}{2}}$, the 3rd through 10th moments in floating point approximations are

$$[0.7810052982, 3.942047050, 9.146681877, 37.12169647, 137.7143092, \\ 613.5286860, 2872.409923, 14709.75560].$$

The same technique can be applied to other variants of Quicksort in this paper and we leave this to interested readers.

6 Future Work and Final Remarks

In such a rich and active research area as Quicksort, there are still several things we could think about to improve the algorithms' performances. Just to name a few, in 2-pivot Quicksort when we compare non-pivot elements with the pivots to determine which sublist they belong to, if the history is tracked, e.g., we already know quite a lot compared elements are smaller than the smaller pivot then it might be better to compare the next element with the larger pivot first. The optimal strategy would vary with the additional information about the range of the numbers or the relative ranking of the two pivots among all the elements.

As for k -pivot Quicksort, our naive approach only distinguishes two cases: whether the currently to-be-sorted list has length less than k or not. If the length is less than k , we use 1-pivot Quicksort, otherwise we still choose k pivots. However, it might be able to improve the performance if the number of pivots varies according to the length of the to-be-sorted list or sublist. Let's say, there is a function $g(n)$, where n is the length of the list. So we

pick $g(n)$ pivots at the beginning. After we obtain the $g(n) + 1$ sublists with length n_i , ($1 \leq i \leq g(n) + 1$), for each one of them, we choose $g(n_i)$ pivots. It would be interesting whether we can find an optimal g in terms of its average performance. Additionally, when k is large, it might make sense to use multi-pivot Quicksort to sort the k pivots as well.

Of course, it is also interesting to study the explicit expressions of the numbers of swaps in multi-pivot Quicksort. But it appears to be dependent on the specific implementation of the algorithm so it is of significance to look for variants which save time and space complexity.

The main results of this paper are those explicit expressions of moments and recurrence relations for either the number of comparisons or the number of swaps of various Quicksort variants. Though all of their asymptotics are $O(n \log n)$, the constant before this term varies a lot and some comparisons of these variants are also discussed. When there is difficulty getting the explicit expressions, numerical tests and Monte Carlo experiments are performed. We also have a demonstration on how to get more moments and find the numeric approximation of the scaled limiting distribution.

Nevertheless, more important than those results is the illustration of a methodology of experimental mathematics. From ansatzes and sufficient data we have an alternative way to obtain results which might be extremely difficult or even impossible to get via traditional human approaches to algorithm analysis. In experimental mathematics we trust.

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