Best-case Analysis of MergeSort
with an Application to the Sum of Digits Problem

A manuscript (MS) intended for future journal publication

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Abstract
An exact formula

\[ B(n) = \frac{n}{2} (\lfloor \lg n \rfloor + 1) - \sum_{k=0}^{\lfloor \lg n \rfloor} 2^k \text{Zigzag}\left(\frac{n}{2^{k+1}}\right), \]

where

\[ \text{Zigzag}(x) = \min(x - \lfloor x \rfloor, \lceil x \rceil - x), \]

for the minimum number \( B(n) \) of comparisons of keys performed by MergeSort
on an \( n \)-element array is derived and analyzed. The said formula is less complex than any other known formula for the same and can be evaluated in \( O(\log c) \) time, where \( c \) is a constant. It is shown that there is no closed-form formula for the above. Other variants for \( B(n) \) are described as well.

Since the recurrence relation for the minimum number of comparisons of keys for MergeSort is identical with a recurrence relation for the number of 1s in binary expansions of all integers between 0 and \( n \) (exclusively), the above results extend to the sum of binary digits problem.

Keywords: MergeSort, sum of digits, sorting, best case.
2010 MSC: 68W40 Analysis of algorithms,
2010 MSC: 11A63 Radix representation
ACM Computing Classification
Theory of computation: Design and analysis of algorithms: Data structures
design and analysis: Sorting and searching
Mathematics of computing: Discrete mathematics: Graph theory: Trees
Mathematics of computing: Continuous mathematics: Calculus

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1. Introduction

“One Picture is Worth a Thousand Words”
[An advertisement for the San Antonio Light (1918)]

Teaching undergraduate Analysis of Algorithms has been a rewarding, although a bit taxing, experience. I was often surprised to learn that many basic problems that clearly belong to its core syllabus had been left unanswered or partially answered. Also, it seemed a bit odd to me that many otherwise decent texts offered unnecessarily imprecise computations\(^1\) of several rather fundamental results.

In this article, I pursue a seemingly marginal topic, the best-case behavior of a well-known sorting algorithm \texttt{MergeSort}, which pursuit, however, yields some interesting findings that could hardly be characterized as “marginal.” It turns out that - contrary to what a casual student of this subject might believe - computing the exact formula for the number of comparisons of keys that \texttt{MergeSort} performs on any \(n\)-element array in the best case is not a routine exercise and leads to a problem that gained some notoriety for being a hard nut to crack analytically: the sum of digits problem. Even more unexpectedly, a relatively straightforward\(^2\) formula for the said number of comparisons yields an improvement of a well-known answer to this instance of the sum of digits problem:

How many 1s appear in binary representations of all integers between (but not including) 0 and \(n\)?

2. \texttt{MergeSort} and its best-case behavior

A call to \texttt{MergeSort} inherits an \(n\)-element array \(A\) of integers and sorts it non-decreasingly, following the steps described below.

\textbf{Algorithm} \texttt{MergeSort} 2.1. \textit{To sort an \(n\)-element array \(A\) do:}

1. If \(n \leq 1\) then return \(A\) to the caller,
2. If \(n \geq 2\) then

\[\text{[Footnotes]}\]
\footnote{1}A notable exception in this category is \([\text{SF13}]\).
\footnote{2}Although not quite \textit{closed-form}.\]
(a) pass the first $\lfloor \frac{n}{2} \rfloor$ elements of A to a recursive call to MergeSort,
(b) pass the last $\lceil \frac{n}{2} \rceil$ elements of A to another recursive call to MergeSort,
(c) linearly merge, by means of a call to Merge, the non-decreasingly sorted arrays that were returned from those calls onto one non-decreasingly sorted array $A'$,
(d) return $A'$ to the caller.

A Java code of Merge is shown on the Figure 1.

```java
private static int[] Merge(int[] A, int[] B)
{
    int[] C = new int[A.length + B.length];
    int indexA = 0, indexB = 0, indexC = 0;
    while ((indexA < A.length) && (indexB < B.length))
    {
        if (A[indexA] < B[indexB] & Bcnt.incr()) // move A[indexA] to C
            C[indexC++] = A[indexA++];
        else // move B[indexB] to C
            C[indexC++] = B[indexB++];
    }
    // copy the remaining part of A or B to C
    if (indexA < A.length) // copy the remaining part of A
        for (int i = indexA; i < A.length; i++)
            C[indexC++] = A[i];
    else // copy the remaining part of B
        for (int i = indexB; i < B.length; i++)
            C[indexC++] = B[i];
    // cnt2.incr();
    return C;
}
```

Figure 1: A Java code of Merge, based on a pseudo-code from [Baa91]. Calls to Boolean method Bcnt.incr() count the number of comps.

A typical measure of the running time of MergeSort is the number of comparisons of keys, which for brevity I call comps, that it performs while sorting array A. Since no comps are performed outside Merge, the running time of MergeSort can be computed as the sum of numbers of comps performed by all calls to Merge during the execution of MergeSort. Since the minimum number of comps performed by Merge on two list is equal to the length of the shorter list, and any increasingly sorted array on any size $N \geq 2$ produces only best-case scenarios for all subsequent calls to Merge, a rudimentary analysis of the recursion tree for MergeSort easily yields the exact formula for the minimum number of comps for the entire MergeSort. The problem arises when one tries to reduce the said formula, which naturally involves long summations, to one that can be evaluated in a logarithmic time.
2.1. Recursion tree

The obvious recursion tree for MergeSort and sufficiently large \( n \) is shown on Figure 2. A recursive application of the equality\(^3\)

\[ \lceil \frac{n}{2} \rceil = \lfloor \frac{n+1}{2} \rfloor \]  

allows for rewriting of that tree onto one whose first four levels are shown on Figure 3.

2.2. Best-case and its characterization \( B(n) \)

The best-case arrays of sizes \( \lceil \frac{n}{2} \rceil \) and \( \lceil \frac{n}{2} \rceil \) for Merge, where \( n \geq 2 \), are those in which every element of the first array is less than all elements of the second one. In such a case, MergeSort performs \( \lceil \frac{n}{2} \rceil \) of comps.

\(^3\)It can be verified separately for odd and even values of \( n \).
Figure 3: The first four levels of the recursion 2-tree $T$ from Figure 2, with the equality (1) applied, recursively. The number of comparisons of keys performed in the best case by \texttt{Merge} invoked in step 2c of Algorithm 2.1 as a result to a call to \texttt{MergeSort} corresponding to a node of $T$ is equal to the number that is shown in its left child, highlighted yellow. All the right children at level $k \geq 1$ of $T$ show numbers of the form $\lfloor \frac{n + i}{2^k} \rfloor$, where $i \geq 2^k$. Thus all the left children (highlighted yellow) at level $k \geq 1$ show numbers of the form $\lfloor \frac{n + i}{2^k} \rfloor$, where $i < 2^k$.

Thus the following recurrence relation for the least number $B(n)$ of comparisons of keys that \texttt{MergeSort} performs on any $n$-element array is straightforward to derive from its description given by Algorithm 2.1:

$$B(1) = 0,$$

and, for $n \geq 2$,

$$B(n) = \left\lfloor \frac{n}{2} \right\rfloor + B\left(\left\lfloor \frac{n}{2} \right\rfloor \right) + B\left(\left\lceil \frac{n}{2} \right\rceil \right).$$

Using the equality (1), the recurrence relation (3) is equivalent to:

$$B(n) = \left\lfloor \frac{n}{2} \right\rfloor + B\left(\left\lfloor \frac{n}{2} \right\rfloor \right) + B\left(\left\lceil \frac{n + 1}{2} \right\rceil \right).$$

A graph of $B(n)$ is shown on Figure 4.

Unfolding the recurrence (4) allows for noticing that the minimum number $B(n)$ of comps performed by all calls to \texttt{Merge} is equal to the sum of all values shown at nodes highlighted yellow in the recursion tree $T$ of Figure 3. They may be summed-up level-by-level. One can notice from Figure 3 that the
number of comps performed at any level \( k \) with the maximal number \( 2^k \) of nodes is given by this formula:

\[
\sum_{i=0}^{2^k-1} \left\lfloor \frac{n+i}{2^{k+1}} \right\rfloor.
\]

(5)

What is not clear is whether all levels of the recursion tree \( T \) are maximal. Fortunately, the answer to this question does not depend on whether given instance of MergeSort is running on a best-case array or on any other case of array. It has been known form a classic analysis of the worst-case running time of MergeSort that every level of its recursion tree \( T \) that contains at least one non-leaf, or - in other words - a node that shows value \( p \geq 2 \), is maximal. Appendix Appendix A page 21 contains a detailed derivation of that fact. Thus all levels 0 through \( h - 1 \) of \( T \) are maximal. Therefore, the formula (5) gives the number of comps for every level \( 0 \leq k \leq h - 1 \).

The last level \( h \) of \( T \) may be not maximal because the level \( h - 1 \) may contain leaves, or - in other words - nodes that show value \( p = 1 \), where \( p = \left\lfloor \frac{n+i}{2^h} \right\rfloor \) for some \( 0 \leq i \leq 2^{h-1} - 1 \), and as such do not have any children in level \( h \). However, for each such node the value of \( \left\lfloor \frac{n+i}{2^h} \right\rfloor \) is 0, so it can be included in summation (5) without affecting its value even though the said value does not correspond to any node in level \( h \). Therefore, the formula (5) gives the number of comps for level \( k = h \).
Also, the depth of $T$ is $\lfloor \log_2 n \rfloor$, as the Theorem A.0.2 in Appendix A states. Thus the minimum number of comps performed by MergeSort is given by this formula:

$$\sum_{k=0}^{\lfloor \log_2 n \rfloor} \sum_{i=0}^{2^k-1} \left\lfloor \frac{n + i}{2^{k+1}} \right\rfloor.$$  \hfill (6)

Unfortunately, the summation (6) contains $n - 1$ non-zero terms, so it cannot be evaluated quickly in its present form. Fortunately, its inner summation (5) can be reduced to a closed-form formula.

### 2.3. Zigzag function

In order to reduce (5) to a closed form, I am going to use function Zigzag defined by:

$$\text{Zigzag}(n) = \min(x - \lfloor x \rfloor, \lceil x \rceil - x).$$  \hfill (7)

The following fact is instrumental for that purpose.

**Theorem 2.2.** For every natural number $n$ and every positive natural number $m$,

$$\sum_{i=m}^{2m-1} \left\lfloor \frac{n + i}{2m} \right\rfloor - \sum_{i=0}^{m-1} \left\lfloor \frac{n + i}{2m} \right\rfloor = 2m \times \text{Zigzag}(\frac{n}{2m}),$$  \hfill (8)

where Zigzag is a function defined by (7) and visualized on Figure 5.

![Figure 5: Graph of function Zigzag(x) = min(x - \lfloor x \rfloor, \lceil x \rceil - x).](image)

*Proof.* The equality (8) can be verified experimentally, for instance, with a help of software for symbolic computation\(^4\). The analytic proof will be published elsewhere. \hfill \square

\(^4\) I used Wolfram Mathematica for that purpose.
Corollary 2.3. For every natural number \( n \) and every positive natural number \( m \),
\[
\sum_{i=0}^{m-1} \left\lfloor \frac{n+i}{2m} \right\rfloor = \frac{n}{2} - m \times \text{Zigzag}\left(\frac{n}{2m}\right),
\] (9)
where Zigzag is a function defined by (7) and visualized on Figure 5.

Proof. First, let’s note\(^5\) that
\[
\sum_{i=0}^{2m-1} \left\lfloor \frac{n+i}{2m} \right\rfloor = n.
\] (10)

From (10) I conclude
\[
\sum_{i=0}^{m-1} \left\lfloor \frac{n+i}{2m} \right\rfloor + \sum_{i=m}^{2m-1} \left\lfloor \frac{n+i}{2m} \right\rfloor = n.
\] (11)

Solving equations (8) and (11) for \( \sum_{i=0}^{m-1} \left\lfloor \frac{n+i}{2m} \right\rfloor \) yields (9). \(\square\)

Here is the closed-form of the summation (5).

Corollary 2.4. For every natural number \( n \) and every natural number \( k \),
\[
\sum_{i=0}^{2k-1} \left\lfloor \frac{n+i}{2k+1} \right\rfloor = \frac{n}{2} - 2^k \text{Zigzag}\left(\frac{n}{2^{k+1}}\right),
\] (12)
where Zigzag is a function defined by (7) and visualized on Figure 5.

Proof. Substitute \( m = 2^k \) in (9). \(\square\)

The following theorem yields the formula (13) for the minimum number \( B(n) \) of comps performed by MergeSort.

Theorem 2.5. For every natural number \( n \),
\[
\sum_{k=0}^{\lfloor \log_2 n \rfloor} \sum_{i=0}^{2^k-1} \left\lfloor \frac{n+i}{2^{k+1}} \right\rfloor = \frac{n}{2} (\lfloor \log_2 n \rfloor + 1) - \sum_{k=0}^{\lfloor \log_2 n \rfloor} 2^k \text{Zigzag}\left(\frac{n}{2^{k+1}}\right),
\] (13)
where Zigzag is a function defined by (7) and visualized on Figure 5.

\(^5\)Analytic proof of that fact is a straightforward exercise; see Appendix B page 25.
Proof.

\[
\sum_{k=0}^{\lfloor \log n \rfloor} \sum_{i=0}^{2^k - 1} \left\lfloor \frac{n + i}{2^{k+1}} \right\rfloor = \sum_{k=0}^{\lfloor \log n \rfloor} \left( \frac{n}{2} - 2^k \text{Zigzag} \left( \frac{n}{2^{k+1}} \right) \right) = \frac{n}{2} (\lfloor \log n \rfloor + 1) - \sum_{k=0}^{\lfloor \log n \rfloor} 2^k \text{Zigzag} \left( \frac{n}{2^{k+1}} \right).
\]

\[\square\]

Figure 6: Graphs of functions \(\sum_{k=0}^{\lfloor \log n \rfloor} \sum_{i=0}^{2^k - 1} \left\lfloor \frac{n + i}{2^{k+1}} \right\rfloor\) (bottom line) and \(\frac{n}{2} (\lfloor \log n \rfloor + 1) - \sum_{k=0}^{\lfloor \log n \rfloor} 2^k \text{Zigzag} \left( \frac{n}{2^{k+1}} \right)\) (top line) of equality (13). They coincide with each other for all natural numbers \(n\).

Formula (13), although not quite closed-form, comprises of summation with only \(\lfloor \log n \rfloor + 1\) closed-form terms, so it may be evaluated in \(O(\log^c)\) time, where \(c\) is a constant. I will show in Section 3 that (13) does not have a closed form. Graphs of both sides of equality (13) are shown on Figure 6. Once can see that for natural numbers \(n\) they coincide with the solution \(B(n)\) of recurrences \(2\) and \(3\) visualized on Figure 4.

**Corollary 2.6.** For every natural number \(n\), the minimum number \(B(n)\) of comps that MergeSort performs while sorting an \(n\)-element array is:

\[
B(n) = \frac{n}{2} (\lfloor \log n \rfloor + 1) - \sum_{k=0}^{\lfloor \log n \rfloor} 2^k \text{Zigzag} \left( \frac{n}{2^{k+1}} \right),
\]

(14)

where Zigzag is a function defined by (7) and visualized on Figure 5.
3. A fractal in \( B(n) \)

A deceitfully simple expression

\[
\sum_{k=0}^{\lfloor \log x \rfloor} 2^{k+1} \text{Zigzag} \left( \frac{x}{2^{k+1}} \right),
\]

(15)

half of which occurs in formula (14) of Corollary 2.6 is a formidable adversary for those who may try to turn it into a closed form, although the time required for its evaluation for any given \( n \) is \( O(\log^c n) \) \(^6\). That does not come as a surprise, taking into account that its graph, shown on Figure 7, bears a resemblance of fractal. This can be easily seen as soon as a sawtooth function \( 2^{\lfloor \log x \rfloor + 1} - x \) is subtracted from it, yielding the function \( F(x) \) given by

\[
F(x) = \sum_{k=0}^{\lfloor \log x \rfloor} 2^{k+1} \text{Zigzag} \left( \frac{x}{2^{k+1}} \right) - 2^{\lfloor \log x \rfloor + 1} + x.
\]

(16)

Figure 7: A graph of function \( \sum_{k=0}^{\lfloor \log x \rfloor} 2^{k+1} \text{Zigzag} \left( \frac{x}{2^{k+1}} \right) \) plotted against a sawtooth function \( 2^{\lfloor \log x \rfloor + 1} - x \).

Since \( \frac{1}{2} \leq \frac{x}{2^{\lfloor \log x \rfloor + 1}} < 1 \), equality (7) implies

\[
\text{Zigzag} \left( \frac{x}{2^{\lfloor \log x \rfloor + 1}} \right) = 1 - \frac{x}{2^{\lfloor \log x \rfloor + 1}},
\]

\(^6\)So, to all practical purposes, (14) is a closed-form formula.
or
\[
2^{\lceil \log x \rceil + 1} \text{Zigzag} \left( \frac{x}{2^{\lceil \log x \rceil + 1}} \right) = 2^{\lceil \log x \rceil + 1} - x. \tag{17}
\]

The equality (17) simplifies definition (16) of function \( F \) to
\[
F(x) = \sum_{k=1}^{\lfloor \log x \rfloor} 2^k \text{Zigzag} \left( \frac{x}{2^k} \right), \tag{18}
\]
visualized on Figure 8.

Figure 8: A graph of function \( F(x) = \sum_{k=1}^{\lfloor \log x \rfloor} 2^k \text{Zigzag} \left( \frac{x}{2^k} \right) \) plotted below its tight linear upper bound \( y = \frac{x-1}{2} \) (if can be shown that \( F(x) = \frac{x-1}{2} \) whenever \( x = \frac{1}{3}(2^k+1+(-1)^k) \) for some integer \( k \geq 0 \)); also shown below \( F(x) \) are the terms \( 2^k \text{Zigzag} \left( \frac{x}{2^k} \right) \) of the summation and their tight linear upper bound \( y = \frac{x}{3} \).

The function \( F \) is a fractal with quasi similarity that repeats at intervals of exponentially growing length. It is a union
\[
F = \bigcup_{k=0}^{\infty} f_k \tag{19}
\]
of functions \( f_k \), each having an interval \([2^k, 2^{k+1})\) as its domain. In other words, for every integer \( k \geq 0 \),
\[
f_k = F \upharpoonright [2^k, 2^{k+1}), \tag{20}
\]
which, of course, yields (19).
Figure 9: A graph of the first six (the first one is 0) normalized parts of function of Figure 8 plotted against the line \( y = \sum_{i=0}^{\infty} \frac{1}{2^{2i+1}} = \frac{2}{3} \). Also shown (in blue) are the first five terms \( \frac{1}{2^i} \text{Zigzag} \left( 2^i x \right) \), \( i = 0, \ldots, 4 \), of sums that occur in the formula (24) for \( \tilde{f}_k(x) \); for each integer \( n \) and all \( x \in [n, n+1) \), their parts above the X-axis restricted to \([n, n+1)\) visualize a fragment of an infinite binary search trie \( T \) defined as the set of shortest binary expansions of \( x - \lfloor x \rfloor \) with the last digit 1 (if the said binary expansion is finite) being interpreted as the sequence terminator; in particular, the root of \( T \) is \( .1 \), and if \( a \) is a finite binary sequence then the children of binary expansion \( .a1 \) are \( .a01 \) and \( .a11 \).

Let \( \hat{f}_k \) be the normalized \( f_k \) on interval \([0, 1)\), defined by:

\[
\hat{f}_k(x) = \frac{1}{2^k} f_k(2^k (x + 1)),
\]  

(21)

and \( \tilde{f}_k \) be the periodized \( \hat{f}_k \) by composing it with a sawtooth function \( x - \lfloor x \rfloor \) defined by:

\[
\tilde{f}_k(x) = \hat{f}_k(x - \lfloor x \rfloor).
\]

(22)

Contracting definitions (20), (21), and (22), yields

\[
\tilde{f}_k(x) = \frac{1}{2^k} F(2^k (x - \lfloor x \rfloor + 1)).
\]

(23)

One can compute\(^7\) from (23) the following alternative formula for \( \tilde{f}_k(x) \):

\[
\tilde{f}_k(x) = \sum_{i=0}^{k-1} \frac{1}{2^i} \text{Zigzag} \left( 2^i x \right).
\]

(24)

\(^7\) The fractional part of \( x \).

\(^8\) An elementary geometric argument based on the graph visualized on Figure 9 will do.
Figure 9 shows functions \( \tilde{f}_0, \ldots, \tilde{f}_6 \) drawn on the same graph.

Since each function \( f_k \), and - therefore - each function \( \tilde{f}_k \), and - therefore - each function \( \tilde{\tilde{f}}_k \), are a result of smaller and smaller triangles piled, originating in function \textit{Zigzag} of definition (18) of function \( F \), on one another as shown on Figure 9, for any integers \( 0 \leq i < j \), \( \tilde{f}_i \) linearly interpolates \( \tilde{f}_j \). Because of that, each \( \tilde{f}_i \) linearly interpolates the limit \( \tilde{F} \) of all \( \tilde{f}_k \)s defined by:

\[
\tilde{F}(x) = \lim_{k \to \infty} \tilde{f}_k(x),
\]

as Figure 10 illustrates. An application of (24) to (25) yields:

\[
\tilde{F}(x) = \sum_{i=0}^{\infty} \frac{1}{2^i} \text{Zigzag} (2^i x).
\]

Since for every integer \( n \) and \( i \geq k \), \( 2^i \frac{n}{2^k} \) is integer, \( \text{Zigzag} (2^i \frac{n}{2^k}) = 0 \). Therefore, by virtue of (24) and (26), for every non-negative integer \( k \) and \( n \),

\[
\tilde{F}(\frac{n}{2^k}) = \tilde{f}_k(\frac{n}{2^k}).
\]

This and (24) eliminate the need for infinite summation\(^9\) while computing \( \tilde{F}(\frac{n}{2^k}) \).

\(^9\)As it appears in (26)
It can be shown that although a continuous function, \( \tilde{F} \) is nowhere-differentiable. As such, it does not have a closed-form formula as any closed-form formula on a real interval must define a function have a derivative at every point of that interval, except for a non-dense set of its points. Since \( \tilde{F} \) can be expressed in function, described by a closed-form formula, of the right-hand side of formula (13), the latter does not have a closed-form formula, either.

**Theorem 3.1.** There is no closed-form formula \( \varphi(n) \) the values of which coincide with \( \sum_{k=0}^{\lfloor \lg n \rfloor} 2^k \text{Zigzag}(\frac{n}{2^{k+1}}) \), for all positive integers \( n \), that is, for every closed-form formula \( \varphi(n) \) on function Zigzag there is a positive \( n \) such that

\[
\sum_{k=0}^{\lfloor \lg n \rfloor} 2^k \text{Zigzag}(\frac{n}{2^{k+1}}) \neq \varphi(n),
\]

where Zigzag is a function defined by (7) and visualized on Figure 5.

**Proof.** Follows from the above discussion.

This way I arrived at the following conclusion.

**Corollary 3.2.** There is no closed-form formula for \( B(n) \).

**Proof.** A closed-form formula for \( B(n) \) would, by virtue of (14) page 10, yield a closed-form formula for \( \sum_{k=0}^{\lfloor \lg n \rfloor} 2^k \text{Zigzag}(\frac{n}{2^{k+1}}) \), which by Theorem 3.1 does not exist.

**Note.** One can apply the reverse transformations to those used in Section 3 on function \( \tilde{F} \) and construct a fractal function \( \check{F} \), shown on Figure 11 given by the equation

\[
\check{F}(x) = 2^{\lfloor \lg x \rfloor} \tilde{F}(\frac{x}{2^\lfloor \lg x \rfloor}),
\]

that for every positive integer \( n \) satisfies

\[
\check{F}(n) = F(n),
\]

where \( F \) is given by (18).
4. Computing $\tilde{F}(x)$ and $B(n)$ from one another

Computing values of function $\tilde{F}(x)$ does not have to be as complex as (or more complex than) the definition (26) implies. Of course, for every integer $n$, $\tilde{F}(n) = 0$. One can apply some elementary arguments based on a structure visualized on Figure 10 to conclude that

$$\tilde{F}\left(\frac{2}{3}\right) = \tilde{F}\left(\frac{1}{3}\right) = \frac{2}{3},$$

(31)

(the latter being the maximum of $\tilde{F}(x)$) or that for every positive integer $k$,

$$\tilde{F}\left(\frac{1}{2^k}\right) = \frac{k}{2^k}.$$ 

(32)

It takes a bit more work to compute

$$\tilde{F}\left(\frac{3}{2^k}\right) = \frac{3k - 4}{2^k}.$$  

(33)

It turns out that computing values of function $\tilde{F}(x)$ for every $x$ that has a finite binary expansion can be done easily if an oracle for computing the values of the function $B(n)$ defined by (2) and (3) is given. Once that is accomplished, since $\tilde{F}(x)$ is a continuous function and the set of numbers with finite binary expansions is dense in the set $\mathfrak{R}$ of reals, it allows for fast approximations of $\tilde{F}(x)$ for every real $x$.

\footnote{Which is not that surprising after a glance at Figure 11.}

\footnote{It helps to remember that $\tilde{F}$ is a periodic function with $\tilde{F}(x) = \tilde{F}(x - \lfloor x \rfloor)$.
Theorem 4.1. For every positive integer \( n \) \(^{12} \) and integer \( k \) with \( n \leq 2^k \),
\[
\tilde{F}(\frac{n}{2^k}) = \frac{n \times k - 2B(n)}{2^k}.
\]

(34)

Proof. The equality (34) can be verified experimentally, for instance, with a help of software for symbolic computation. The analytic proof will be published elsewhere.

Theorem 4.1 allows for easy computing of \( B(n) \) if \( \tilde{F}(\frac{n}{2^k}) \) is given for some \( k \geq \lfloor \lg n \rfloor \) using this form of (34):

Corollary 4.2. For every positive integer \( n \) and integer \( k \) with \( n \leq 2^k \),
\[
B(n) = \frac{n \times k}{2} - 2^{k-1} \tilde{F}(\frac{n}{2^k}).
\]

(35)

Proof. An obvious conclusion from (34).

For instance, putting \( k = \lfloor \lg n \rfloor + 1 \) in (35) easily yields (14). For \( k = \lfloor \lg n \rfloor \) we obtain
\[
B(n) = \frac{n \lfloor \lg n \rfloor}{2} - 2^{\lfloor \lg n \rfloor - 1} \tilde{F}(\frac{n}{2^{\lfloor \lg n \rfloor}}) = \]
\[
\frac{n \lfloor \lg n \rfloor}{2} - 2^{\lfloor \lg n \rfloor - 1} \sum_{i=0}^{\infty} \frac{1}{2^i} \text{Zigzag} (\frac{n}{2^{\lfloor \lg n \rfloor}}) = \]
\[
\frac{n \lfloor \lg n \rfloor}{2} - 2^{\lfloor \lg n \rfloor - 1} \sum_{i=0}^{\lfloor \lg n \rfloor - 1} \frac{1}{2^i} \text{Zigzag} (\frac{n}{2^{\lfloor \lg n \rfloor}}) = \]
\[
\frac{n \lfloor \lg n \rfloor}{2} - \frac{1}{2} \sum_{i=0}^{\lfloor \lg n \rfloor - 1} 2^{\lfloor \lg n \rfloor - i} \text{Zigzag} (\frac{n}{2^{\lfloor \lg n \rfloor - i}}).
\]

Substituting \( k \) for \( \lfloor \lg n \rfloor - i \) we conclude
\[
B(n) = \frac{n \lfloor \lg n \rfloor}{2} - \frac{1}{2} \sum_{k=1}^{\lfloor \lg n \rfloor} 2^k \text{Zigzag} (\frac{n}{2^k}),
\]

(36)
a similar to (14) characterization of \( B(n) \).

\(^{12}\)Of course, one is free to assume that \( n \) is odd here.
5. Relationship between the best case and the worst case

A casual student of MergeSort tends to believe that its worst-case behavior is about twice as bad as its best-case behavior. This, of course, is only approximately true. In this Section, I will derive the exact difference between $2B(n)$ and $W(n)$ using function $F$ defined by (16) page 11.

An exact formula for the number $W(n)$ of comparisons of keys performed by MergeSort in the worst case is known\(^{13}\) and is given for any positive integer $n$ by the following equality:

$$W(n) = \sum_{i=1}^{n} \lceil \log i \rceil.$$  \hspace{1cm} (37)

From (14) and (16), one can derive

\begin{align*}
2B(n) &= n \lfloor \log n \rfloor - 2^{\lfloor \log n \rfloor + 1} + 2n - F(n) = \\
&= \sum_{i=1}^{n} \lfloor \log i \rfloor - 1 + n - F(n) = \\
&= W(n) - 1 + n - F(n).
\end{align*}

The above yield the following characterization.

**Theorem 5.1.** For every positive integer $n$, the difference between twice the number $B(n)$ of comparison of keys performed in the best case and the number $W(n)$ of comparison of keys performed in the worst case by MergeSort while sorting an $n$-element array is:

$$2B(n) - W(n) = n - 1 - F(n),$$  \hspace{1cm} (38)

where $F(n)$, visualized on Figure 8, is given by (18).

**Proof.** Follows from the above discussion. \hfill \square

\(^{13}\)See (A.7) in the Appendix A.
In particular, since for every positive integer \( n \),
\[
0 \leq F(n) \leq \frac{n - 1}{2}
\]  
(see Figure 8 for explanation), I conclude with the following tight linear bounds on \( 2B(n) - W(n) \).

**Corollary 5.2.** For every positive integer \( n \), the difference between twice the minimum number \( B(n) \) and the maximum number \( W(n) \) of comparison of keys performed in the worst case by MergeSort while sorting an \( n \)-element array satisfies this inequality:
\[
\frac{n - 1}{2} \leq 2B(n) - W(n) \leq n - 1.
\]  
(40)

**Proof.** Follows from (38) and (39).  

![Figure 12: A graph of \( 2B(n) - W(n) \) shown between graphs of its tight linear bounds \( n - 1 \) and \( \frac{n - 1}{2} \).](image)

Obviously, \( 2B(n) - W(n) = n - 1 \) whenever \( F(n) = 0 \), that is, whenever 
\[
n = 2^{\lfloor \log n \rfloor}.
\]  
It can be shown that \( 2B(n) - W(n) = \frac{n - 1}{2} \) whenever 
\[
n = \frac{1}{3}(2^{k+1} + (-1)^k)
\]  
for some integer \( k \geq 0 \).

A graph of \( 2B(n) - W(n) \) and its tight bounds are shown on Figure 12.
6. The sum of digits problem

A known explicit formula, published in [Tro68], for the total number of bits in all integers between 0 and \( n \) (not including 0 and \( n \)) is expressed in terms of function \( \text{Zigzag} \) (referred to as \( 2g \) in [Tro68]) and is given by:

\[
A(n, r) \equiv \sum_{\sigma \leq n} a(\sigma, r) = \frac{1}{2}(r - 1)n \log_2 n - E(n, r)
\]

Let \( g(x) \) be periodic of period 1 and defined on \([0, 1]\) by:

\[
g(x) = \begin{cases} 
\frac{1}{2}x & 0 \leq x \leq \frac{1}{2} \\
\frac{1}{2}(1 - x) & \frac{1}{2} < x \leq 1.
\end{cases}
\]

The function

\[
f(x) = \sum_{i=0}^{\infty} \frac{1}{2^i} g(2^ix)
\]

can be shown to be nondifferentiable. The relation between this function and \( E(n, 2) \) is demonstrated in the following theorems:

**Theorem 1.** If the integer \( n \) is written \( n = 2^m(1 + x), \ 0 \leq x < 1 \), then

\[
E(n, 2) = 2^{m-1} \{ 2f(x) + (1 + x) \log_2 (1 + x) - 2x \}.
\]

It has been shown in [McI74] that the recurrence relation for \( A(n, 2) \) is the same as the recurrence relation for \( B(n) \) given by (2) and (3). Therefore, the formula (13) derived in this paper is equivalent to \( A(n, 2) \) given above by the considerably more complicated definition. Interestingly, the above definition can be simplified to (13) along the lines of the elementary derivation of the alternative formula (36) for \( B(n) \) on page 17.

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[Baa91] Sara Baase. *Computer Algorithms: Introduction to Design and Analysis*. Addison-Wesley Publishing, 2nd edition, 1991.

[Knu97] Donald E. Knuth. *The Art of Computer Programming*, volume 3. Addison-Wesley Publishing, 2nd edition, 1997.

\[\text{14} \text{The following are screen shots and an excerpt from [Tro68].}\]

\[\text{15} \text{Even more interestingly, if someone did bother to simplify Trollope's formula of [Tro68] then I am not aware of it.}\]
APPENDIX

Appendix A. A derivation of the worst-case running time $W(n) = \sum_{i=1}^{n} \lceil \lg i \rceil$ of MergeSort

Let’s assume that $n \geq 2$ is large enough to spur a cascade of many recursive calls to MergeSort following the recursion tree $T$, a sketch of which is shown on Figure 2.

The nodes in tree $T$ correspond to calls to MergeSort and show sizes of (sub)arrays passed to those calls. The root corresponds to the original call to MergeSort. If a call that is represented by a node $p$ executes further recursive calls to MergeSort then these calls are represented by the children of $p$; otherwise $p$ is a leaf. Thus, $T$ is a 2-tree.$^{16}$

The levels in tree $T$ are enumerated from 0 to $h$, where $h$ is the number of the last level of the tree, or - in other words - the depth of $T$. On Figure 2 they are shown on the left side of the tree. The root is at the level 0, its children are at level 1, its grand children are at level 2, its great grand children (not shown on the sketch) are at level 3, at so on. Clearly, since every call to MergeSort on a sub-array of size $\geq 2$ executes two further recursive calls to MergeSort, only the nodes that show value 1 are leaves and all other nodes have 2 children each. Thus, since all nodes in the last level $h$ are leaves, they all show value 1. And since the original input array gets split, eventually, onto $n$ 1-element sub-arrays, the number of all leaves in $T$ is $n$. (This, however, does not mean that the last level $h$ necessarily contains all the leaves of $T$.)

$^{16}$A binary tree whose every non-leaf has exactly 2 children.
If a level \( i \) has \( 2^i \) nodes, each of them showing a value \( \geq 2 \), then each such node has 2 children so that level \( i + 1 \) has twice the number of nodes in level \( i \), that is, \( 2^{i+1} \) nodes. Since level 0 has \( 2^0 \) nodes, it follows (completion of a proof by induction with the basis and inductive steps outlined above is left as an exercise for the reader) that if \( k \) is the level number of any level above which all the nodes show values \( \geq 2 \) then all levels \( i = 0, \ldots, k \) contain exactly \( 2^i \) nodes each.

The last level \( h \) may contain \( 2^h \) nodes or less. We are going to show that each level \( i \) above level \( h \) contains exactly \( 2^i \) nodes. Here is a very insightful property that we are going to use for that purpose. It states that \texttt{MergeSort} is splitting its input array fairly evenly so that at any level of the recursive tree, the difference between the lengths of the longest sub-array and the shortest sub-array is \( \leq 1 \). This fact is the root cause of good worst-case performance of \texttt{MergeSort}.

**Property Appendix A.0.1.** The difference between values shown by any two nodes in the same level of the recursion tree for \texttt{MergeSort} is \( \leq 1 \).

**Proof.** The Property clearly holds for level 0. We will show that if it holds for level \( i \) and \( i \) is not the last level of the recursion tree (that is, \( i < h \)) then it also holds for the level \( i + 1 \).

Let us assume that the Property holds for some level \( i < h \). Let \( c \leq d \) be numbers shown by any two (not necessarily distinct) nodes in level \( i + 1 \). It suffices to show that

\[ d - c \leq 1. \]  

(A.1)

Let \( a \leq b \) be the numbers shown by the parents of the mentioned above nodes. Those parents, of course, must reside in the level \( i \). By the inductive hypothesis (that holds for level \( i \)), \( b - a \leq 1 \), that is,

\[ a \leq b \leq a + 1. \]  

(A.2)

The numbers shown by all their four children are \( \lfloor \frac{a}{2} \rfloor \), \( \lceil \frac{a}{2} \rceil \), \( \lfloor \frac{b}{2} \rfloor \) and \( \lceil \frac{b}{2} \rceil \), respectively, so the largest difference between any of those four numbers is \( \lfloor \frac{b}{2} \rfloor - \lfloor \frac{a}{2} \rfloor \). In particular, \( d - c \) is not larger than that. We have:

\[ d - c \leq \lfloor \frac{b}{2} \rfloor - \lfloor \frac{a}{2} \rfloor \leq \]

[by (A.2)]

\[ \leq \lfloor \frac{a + 1}{2} \rfloor - \lfloor \frac{a}{2} \rfloor \]
[since for any integer \( c \), \( \lceil \frac{c+1}{2} \rceil \)]

\[
= \left\lfloor \frac{a+2}{2} \right\rfloor - \left\lfloor \frac{a}{2} \right\rfloor = \left\lfloor \frac{a}{2} + 1 \right\rfloor - \left\lfloor \frac{a}{2} \right\rfloor
\]

[since for every \( x \), \( \lfloor x + 1 \rfloor = \lfloor x \rfloor + 1 \)]

\[
= \left\lfloor \frac{a}{2} \right\rfloor + 1 - \left\lfloor \frac{a}{2} \right\rfloor = 1.
\]

Thus (A.1) holds. This completes the inductive step and completes the proof of the Property.

As we have noted, the values shown at all nodes in the last level \( h \) are all 1. Thus the values shown at their parents, that reside at level \( h - 1 \) are all 2, and the values shown at their grand parents, that reside at level \( h - 2 \) are all \( \geq 3 \). Thus, by Property Appendix A.0.1 all nodes at level \( h - 2 \) show values \( \geq 2 \), and, therefore (as we have proved before), all levels \( i = 0, ..., h - 1 \) have \( 2^i \) nodes, each, as it has been visualized on Figure 2.

**Theorem Appendix A.0.2.** The depth \( h \) of the recursion tree \( T(n) \) for MergeSort run on an array of size \( n \) is

\[
h = \lfloor \lg n \rfloor.
\]  

\[ (A.3) \]

**Proof.** Since every level of \( T \), except, perhaps, for the last level, has the maximal number of nodes, a 2-tree with \( n \) leaves could not be any shorter than \( T \). So, \( T \) is a shortest 2-tree with \( n \) leaves. Therefore (by a well known fact), its depth \( h \) is equal to \( \lfloor \lg n \rfloor \). Thus (A.3) holds.

Because each node in any level above \( h - 1 \) shows value \( \geq 2 \), it has 2 children. Thus the value it shows is equal to the sum of values shown by its children, as we have indicated at the beginning of this section. From that we conclude (a proof by induction is left as an exercise for the reader) that the sum of values shown at nodes in any level \( i = 0, ..., h - 1 \) is the same for each such level. Thus the said sum is equal to the value showed by the only node at level 0, that is, is equal to \( n \).

Let \( a_1, ..., a_{2^i} \) be the values shown at the nodes of some level \( i = 0, ..., h - 1 \). The number of comps performed by a call to Merge invoked by the call to MergeSort on an array of \( a_j \) elements is either 0 if \( a_j = 1 \) (no call to Merge
is made) or, as we have shown in the previous section, is \( a_j - 1 \) if \( a_j \geq 2 \). So, in either case, it is \( a_j - 1 \). Thus the number of comps \( C_i \) performed at level \( i \) is

\[
C_i = (a_1 - 1) + \ldots + (a_{2^i} - 1) = (a_1 + \ldots + a_{2^i}) - (1 + \ldots + 1) = n - 2^i. \quad (A.4)
\]

Moreover, since all nodes at the last level \( h \) are 1’s

\[
C_h = 0. \quad (A.5)
\]

Therefore, the total number \( W(n) \) of comps that \texttt{MergeSort} performs in the worst case on an \( n \)-element array is equal to

\[
W(n) = \sum_{i=0}^{h} C_i =
\]

[by (A.5)]

\[
= \sum_{i=0}^{h-1} C_i =
\]

[by (A.4)]

\[
= \sum_{i=0}^{h-1} (n - 2^i) = nh - (2^h - 1) = nh - 2^h + 1 =
\]

[by (A.3)]

\[
= n \lceil \log n \rceil - 2^\lceil \log n \rceil + 1.
\]

This way I have proved the following.

**Theorem Appendix A.1.** The number \( W(n) \) of comparisons of keys that \texttt{MergeSort} performs in the worst case while sorting an \( n \)-element array is

\[
W(n) = n \lceil \log n \rceil - 2^\lceil \log n \rceil + 1. \quad (A.6)
\]

**Proof** follows from the above derivation. \( \square \)

Using the well-known\(^{17}\) closed-form formula for \( \sum_{i=1}^{n} \lceil \log i \rceil \), I conclude that

\[
W(n) = \sum_{i=1}^{n} \lceil \log i \rceil. \quad (A.7)
\]

\(^{17}\text{See [Knu97].}\)
Appendix B. Proof of $\sum_{i=0}^{m-1} \lfloor \frac{n+i}{m} \rfloor = n$

**Theorem Appendix B.0.3.** For every natural number $n$ and every positive natural number $m$,

$$\sum_{i=0}^{m-1} \lfloor \frac{n+i}{m} \rfloor = n.$$  

**Proof.** Let $n = km + l$, where $0 \leq l < m$.

We have

$$\lfloor \frac{n+i}{m} \rfloor = \lfloor \frac{km+l+i}{m} \rfloor = \lfloor k + \frac{l+i}{m} \rfloor = k + \lfloor \frac{l+i}{m} \rfloor.$$

Therefore,

$$\sum_{i=0}^{m-1} \lfloor \frac{n+i}{m} \rfloor = mk + \sum_{i=0}^{m-1} \lfloor \frac{l+i}{m} \rfloor = mk + \sum_{i=m-l}^{m-1} \lfloor \frac{l+i}{m} \rfloor = mk + \sum_{i=m-l}^{m-1} 1 = mk + l = n.$$  

\[\square\]

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[Tro68] J. R. Trollope. An explicit expression for binary digital sums. *Mathematics Magazine*, 41(1):21–25, Jan.–Feb. 1968.

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