COMP20012: An Introduction to Algorithms and Data Structures

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<u>Overview</u>

Aims

This course is an introduction to the design, analysis and wide variety of algorithms (a topic often called 'Algorithmics').

We shall look at the specification of computational tasks, varieties of algorithms for tasks, demonstrating (through informal proof) that algorithms perform given tasks, the structure of algorithms and, finally, measures for comparing the performance of algorithms.

We also consider the implementation of algorithms and relevant data and program structures, and principles of program design.

Contents

- 1. Idea of Algorithms: algorithms and programs. Some history. Formalising algorithms, programming languages and machine models.
- 2. Specification and correctness. Informal correctness proofs.
- 3. Performance of algorithms. The issues. Performance measures. Complexity: Counting, worst- best- and average-cases. Recurrence relations for computing complexity. Asymptotic approximation.
- 4. Searching and sorting algorithms.
- 5. Trees and graphs and associated algorithms.
- 6. Hashing

Organisation

The module is in two sections. Section (1) is taught by David Rydeheard; Section (2) by Graham Gough.

The website

You should all consult the website for this module. It contains (1) all the lecture notes and slides, (2) ALL TUTORIAL SHEETS, (3) relevant code, (4) details of module organisation, (5) useful links to many other relevant sites, including good algorithm sites.

<u>Books</u>

The course textbook is:

Mark Allen Weiss, Data Structures. Problem Solving using JAVA (ISBN 0-201-74835-5) Addison-Wesley. 2001.

This is a high quality book in the area. The lectured material is based on this textbook. You are all recommended to get access to it.

Background Reading: Good support textbooks are:

- SEDGEWICK, R. Algorithms in C (ISBN 0-201-51425-7) Addison-Wesley 1990. A general, good quality, book on algorithms, with very good detail.
- CORMEN, T. H. et al, Introduction to Algorithms, (ISBN 0-262-530-910) MIT Press 1994. This is an encyclopaedic reference, well written and extremely thorough.

• HAREL, D. Algorithmics; the Spirit of Computing 2nd Edition, Addison Wesley 1992. A good informal (and readable) introduction to the subject.

You are also urged to consult some of the classic texts in the area, chief of which is: Knuth, D. E. Fundamental Algorithms, Addison Wesley 1968.

Algorithms

- What are they? Not really a defined idea. Informally, a recipe, or procedure, or construction; algorithms themselves consist of precise descriptions of procedures.
- The word: It's history lies in Arabicized Persian, from al-Kuwarizmi ('the man from Kuwarizm' modern-day Khiva, in Uzbekistan, south of the Aral Sea), the mathematician Abu Ja'far Muhammad ibn Musa (c780-c850 living in Baghdad) who wrote Hisab al-Jabr wa'l-muqabala ('Rules for restoring and equating').

The European translation of his works introduced the Hindu-Arabic notation for numbers. This is our standard notation for numbers: 124 means 1 hundred, 2 tens and 4 units! It is *positional* (Hindu) and has a *zero* (Arabic). The standard algorithms for arithmetic are expressed in this *notation*.

Complexity of Algorithms (Chapter 5 of textbook)

Idea: We want to *compare* the *performance* of different algorithms for a given task in terms of some *measure of efficiency*.

For example: We may want to find 'how long an algorithm (coded as a program) takes to compute a result'.

But: This varies with (1) program code, (2) programming language, (3) compiler, (4) processor etc (operating system, weather...). Time itself is not a useful measure.

We seek: Measures that are *intrinsic* to an algorithm (ie independent of all the conditions above), but nevertheless give a real assessment of the performance of algorithms.

Complexity measures

Such measures are called *complexity measures* and consist simply of counting, as follows:

Two common measures

- The **TIME COMPLEXITY** of an algorithm consists of a count of the number of *time-critical operations* as the *size of the input* varies.
- The **SPACE COMPLEXITY** of an algorithm consists of a count of the number of *space cells* as the *size of the input* varies.

The choice of which operations are time critical and what constitutes a space cell, varies according to application, as we shall see.

NB Complexity is about performance measures, NOT about the intricacy of programs.

Worst-case, best-case and 'average-case' measures

Suppose we are given an algorithm and we wish to assess its performance on inputs of size N. Usually, even with inputs of a fixed size, the performance can vary considerably according to the contents of the input and the arrangement of data.

However, we can identify:

- The **best-case** performance for each size N the smallest time complexity (or space complexity) over all inputs of size N.
- The worst-case performance for each size N the largest time complexity (or space complexity) over all inputs of size N.

These are extremal measures, and we would like to be able to assess the performance on average, but this is more difficult to compute as we shall see.

An Example: Searching

TASK: Given

- an item, and
- a sequence/list of items

find whether or not the item occurs in the sequence.

[Part of a family of problems: find all occurrences, find number of occurrences, find first occurrence etc.]

Algorithm 1: Sequential search

If sequence empty then stop with failure. Otherwise, compare given item with head of sequence, using equality test. If found then stop with success, else continue down tail of sequence, successively testing for equality, until success or sequence becomes empty.

Performance

The performance of this algorithm clearly varies with the length of the sequence. Let N be the length.

For time complexity, which operation is 'time critical'? Usually, it is the *equality test* of the item against members of the sequence.

[An alternative is the operation of access to the sequence, but for this algorithm each access is followed by one equality test so they are equivalent.]

Given a sequence of length N, how many equality tests are performed?

• If the item sought is found at the head of the sequence then 1 equality test only is required:

Best-case time complexity = 1. This is constant i.e. independent of N.

• If the item sought is found at the end of the sequence or is not in the sequence then N equality tests are required:

Worst-case time complexity = N. This is linear.

The best-case is the *lower bound* and the worst case is the *upper bound* of any actual performance.

'Average-case' time complexity

Is either of these - the best-case or the worst-case - a realistic measure of what happens on average?

Let us try to define average-case time complexity.

This is a difficult concept and often difficult to compute. It involves probability and infinite distributions.

What is an average sequence of integers? If all integers are equally probable in the sequence then the probability that any given integer is in the sequence is zero! (Probability zero does not mean impossible when there are infinite distributions around.)

For sequential search on sequences of random integers this means

Average-case time complexity = N. This is *linear* and the same as worst-case.

Note: The average case is NOT the average of the best-case and worst-case, but is an average over all possible input sequences and their probabilities of occurrence.

If the sought item is known to occur exactly once in the sequence and we seek its position, then the average case is N/2.

Algorithm 2: Binary Search (Chapter 7 of textbook)

Suppose the items in the sequence are integers - or any type with a given (total) order relation \leq on it - and the sequence is already in ascending (i.e. non-descending) order. Binary search is:

- 1. If the sequence is empty, return false.
- 2. If the sequence contains just one item, then return the result of the equality test.
- 3. Otherwise: compare given item with a 'middle' item:
 - If equal, then return success.
 - If given item is less than middle item, then recursively call binary search on the sequence of items to the left of the chosen middle item.
 - If given item is greater than middle item, then recursively call binary search on the sequence of items to the right of the chosen middle item.

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Program: Could write this recursively, as suggested, or iteratively
as below.
public static int binarysearch( Comparable [] seq,
                                  Comparable item )
   int left = 0; int right = seq.length -1;
   int middle, comparison;
   while (left <= right)</pre>
    { middle = (left+right)/2;
      comparison = seq[middle].compareTo(item);
      if (comparison == 0) return middle;
      else if (comparison < 0) right = middle-1;
      else left = middle+1;
   return -1;
```

Note

- The use of Comparable class and compareTo method to capture the genericity of the algorithm. The comparison here is a three way comparison, including equality, but other forms are possible. The algorithm returns either −1 for false, or the position of the first found occurrence.
- The need for arrays, rather than, say linked lists, because we need 'random access' i.e. access to all parts (esp middle item) in constant-time. Compare sequential search where either arrays or linked lists would be appropriate.

Correctness of binary search

The argument for the correctness of the algorithm goes as follows: Suppose we seek an item in a sequence of length N. We proceed by induction on N.

If N = 0 then the algorithm returns -1 (false) as required.

Otherwise, suppose the algorithm is correct on all ascending sequences of length less than N. If we can show it is correct on all ascending sequences of length N, then by induction, it is correct for all finite ascending sequences.

On an ascending sequence of length N, it first selects an item (the 'middle' item) and compares it with the given item, if equal it returns the position, as required.

If not equal, then because the sequence is in ascending order, if the item sought is less than the middle item, then it can only occur in the left subsequence, which itself is an ascending subsequence, but

of length at least 1 less than N, so by induction it will correctly find the item, or return false. Similarly, for the case when the item is greater than the middle item.

Induction is a characteristic method for iterative and recursive algorithms as it allows us to establish that something holds assuming that the remaining part of the computation - the recursive call, or remaining loop computation - is correct.

Notice that correctness depends upon the ascending order, but NOT on which element is chosen as the 'middle' element (in fact any element would do for correctness).

Performance of binary search: time complexity

We count the number of *comparisons*.

The algorithm is recursive. How do we count the number of operations in a recursive algorithm?

Either: unfold a few recursive calls and look for a pattern to establish itself, or, equivalently, use recurrence relations.

The worst case is when each attempt to match to a middle element fails and we then approximately half the task. This is the key observation. If we continue halving at each test until one or no elements is left, how many tests are required?

Suppose the list is of length 2^M . The first test failing means that we search in a sequence of length approximately $2^M/2 = 2^{M-1}$. So approximately M+1 comparison tests are required in the worst case.

Logarithmic performance

In general, for sequence length N, how many tests are required in the worst case?

That is, how often do we need to halve the sequence to end up with the final test?

The answer is approximately $\log_2(N)$.

Reminder: The logarithm to base 2 of a number N is the power of 2 which equals N. Thus

$$2^{\log_2(N)} = N.$$

In general, the logarithm is defined by: $A^{\log_A(B)} = B$.

Arithmetic with logarithms

The following rules hold for logarithms (all direct from the definition):

$$\log_A(A) = 1$$
, $\log_A(B \times C) = \log_A(B) + \log_A(C)$

$$\log_A(1/B) = -\log_A(B), \ \log_B(C) = \log_B(A) \times \log_A(C).$$

The second rule above is that for which logarithms were developed - doing multiplication by addition. The final rule allows us to change base of logarithms by multiplying by a constant.

Logarithms (continued)

Logarithms grow much, much slower that linear - so an algorithm that performs logarithmically is, in general, *very fast*:

Linear performance: If the input size doubles, the complexity doubles.

Logarithmic performance: If the input size doubles, the complexity increases by 1!

Other common measures are quadratic N^2 , and exponential 2^N .

Input size	Logarithmic	Linear	Quadratic	Exponential
10	4	10	100	1024
20	5	20	400	10^{6}
100	7	100	10,000	10^{30}
1,000	10	1000	1,000,000	10^{300}
10,000	14	10,000	100,000,00	10^{3000}

Thus binary search is very efficient even in the worst case (we can picture this by saying that half of the material is disposed at each test without looking at it).

It is also very space efficient. It can be implemented *in-place* - without the need for space in addition to that occupied by the input. However, it does need the input to be in ascending order.

Recurrence relations (Chapter 7 of textbook)

... are a general method of calculating the complexity of *recursive* and *iterative* algorithms.

As an example, consider binary search. We introduce the notation that C_N is the number of comparison operations on input of size N in the worst case.

How do we calculate C_N ?

Looking at the algorithm, we see that in the worst case, the number of operations on input size N is 1 (the equality test with the middle element) and then a worst case search on input size approximately N/2.

We can this write

$$C_N = C_{N/2} + 1$$

for N > 0, and for $C_0 = 0$.

This is called a **recurrence relation**. It is a recursive expression for a numerical quantity, computing complexity measures by following the recursive structure of an algorithm.

(Notice that there is some approximation going on here which we will discuss later.)

Recurrence relations have **solutions**.

Sometimes more than one, sometimes one, sometimes none. The cases we deal with derived for computing the complexity of algorithms have *unique solutions* (or a unique family of solutions).

The solution of the above recurrence relation is

$$C_N = \log_2(N) + 1.$$

We can see this simply by substituting:

Left-hand side is $\log_2(N) + 1$.

Right-hand side is
$$C_{N/2}+1=(\log_2(N/2)+1)+1=\log_2(N\times 1/2)+1+1=\log_2(N)+\log_2(1/2)+1+1=\log_2(N)-\log_2(2)+1+1=\log_2(N)-1+1+1=\log_2(N)+1.$$

Hence left-hand and right-hand sides are equal, as required.

(Note: in fact, $\log_2(N) + A$ for any constant A is a solution, but base cases determine that A = 1).

Finding solutions

Given a solution, we can check it. But our task is to find solutions of recurrence relations. How do we do this?

A simple approach is to *expand* the recurrence and see what happens:

$$C_N = C_{N/2} + 1 = (C_{N/4} + 1) + 1 = ((C_{N/8} + 1) + 1) + 1 = \dots = C_1 + 1 + 1 + \dots + 1$$

where there are $\log_2(N)$ number of 1's. Hence $C_N = \log_2(N) + 1$ as required.

In general, algorithms which halve the input at each step have complexity in terms of logarithms base 2 (if a third at each step then log base 3 etc).

Later we look at a range of commonly occurring recurrence relations and we give their solutions.

Algorithm complexity: Approximation and rates of growth

In the above analysis we have used approximations: Saying 'divided approximately in half' and even using $\log_2(N)$ (which in general is not an integer), rather than $\operatorname{ceiling}(\log_2(N))$ (the least integer above $\log_2(N)$.

Why is this?

It is because we are usually only concerned with the *rate of growth* of the complexity as the input size increases.

Complexity (that is the number of operations undertaken) at a fixed size of input, does NOT in general convert to a running time for an algorithm. However, if the operations are chosen correctly, then the rate of growth of the complexity WILL correspond to the rate of growth of the running time.

Rate of growth of numerical expressions

• For complexity $\log_2(N) + 1$ is the 1 significant? No. Whatever the constant is, if the input size doubles the complexity increases by 1.

For small N, the constant is a significant part of the complexity, so that $\log_2(N) + 1$ and $\log_2(N) + 10$ are different, but as N increases the constant looses its significance.

- For complexity $N^2 + 1000 \times N + 123456$ as N increases so does the role of the N^2 part, and the expression grows like N^2 for large N.
- For $N + 1000 \times \log_2(N)$ only the linear term N is significant for large N.

In general, for 'small' N the behaviour of an algorithm may be erratic, involving overheads of setting up data structures, initialization, small components of the complexity, different operations may be important, etc.

We are interested in the rate of growth of expressions as N increases, i.e. what happens at 'large' N?

When N doubles:

- $\log_2(N)$ increases by 1
- $123 \times N$ doubles
- $12 \times N^2$ quadruples (×4)
- $2 \times N^3$ increases eightfold
- 2^N squares (because $2^{2 \times N} = (2^N)^2$)

Exponential algorithms are infeasible - they cannot be run on substantial inputs to provide results. Note: Exponential includes factorial N!

When N doubles, what happens to $N^2 + 1000 \times N + 123456$?

For 'small' N it is approximately constant (because 123456 is big!).

For 'intermediate' N it is linear (because $1000 \times N$ dominates over N^2)

But eventually N^2 dominates the other terms and the behaviour becomes closer to quadratic as N increases.

We introduce a notation for this and say that

$$N^2 + 1000 \times N + 123456$$

is $O(N^2)$ (Oh, not zero!) and read this as the expression is **of** order N^2 . This is called BIG-OH notation.

Defining order of growth

Definition

A function f(N) is of order g(N), written f(N) is O(g(N)), just when there is a constant c such that, for all N sufficiently large

$$f(N) \le c \times g(N)$$

i.e. $\exists c. \exists N_0. \forall N \geq N_0. f(N) \leq c \times g(N)$.

We say g(N) eventually dominates f(N).

Examples

- 1. $3 \times N^2$ is $O(N^2)$
- 2. $N \times \log_2(N) + N + 1$ is $O(N \times \log_2(N))$
- 3. $\log_3(N)$ is $O(\log_2(N))$ because $\log_3(N) = \log_3(2) \times \log_2(N)$
- 4. N^3 is $O(10 \times N^3 + N)$
- 5. N^2 is $O(N^3)$

Recurrence relations and their solutions

Some recurrence relations

• $C_N = C_{N/2} + a$ where a is a constant.

'Do constant amount of work and then halve the remainder' Solution: $C_N = O(\log N)$.

• $C_N = C_{N-1} + a$ where a is a constant.

'Do constant amount of work and then repeat on input of size one less'

Typically, this is a simple loop with a constant amount of work per execution. Example: sequential search.

Solution: $C_N = O(N)$.

• $C_N = C_{N-1} + a \times N$ where a is a constant.

'Do amount of work proportional to N and then repeat on input of size one less'

Typically, two *nested* loops.

$$C_N = C_{N-1} + a \times N = C_{N-2} + a \times (N-1) + a \times N = C_{N-3} + a \times ((N-2) + (N-1) + N) = a \times \frac{N \times (N+1)}{2}$$

Solution: $C_N = O(N^2)$ is quadratic.

Examples: Long multiplication of integers, Bubblesort.

• $C_N = 2 \times C_{N/2} + a \times N$ where a is a constant.

'Do work proportional to N then call on both halves of the input'

[Picture]

Solution: $C_N = O(N \times \log N)$. This is called LinLog behaviour (linear-logarithmic).

• $C_N = C_{N-1} + a \times N^2$ where a is a constant.

'Do amount of work proportional to N^2 and then repeat on input of size one less'

Typically, three *nested* loops.

Solution: $C_N = O(N^3)$ is cubic.

Example: The standard method of matrix multiplication.

• $C_N = 2 \times C_{N-1} + a$ where a is a constant.

'Do constant amount of work and then repeat on two versions of input of size one less'

Solution: $C_N = O(2^N)$ - exponential.

• $C_N = N \times C_{N-1} + a$ where a is a constant.

Solution: $C_N = O(N!) = O(N^N)$ - highly exponential.

(Note: Stirling's approximation $N! \approx \sqrt{2\pi N} (N/e)^N$.)

Infeasible Algorithms

Algorithms with complexities

$$O(1), O(N), O(N^2), O(N^3), O(N^4) \dots$$

and between are called **polynomial**, and are considered as *feasible* - ie can be run on 'large' inputs (though, of course, cubic, quartic etc can be very slow).

Exponential algorithms are called infeasible and take considerable computational resources even for small inputs (and on large inputs can often exceed the capacity of the known universe!).

Examples of Infeasible Algorithms

... are often based on **unbounded exhaustive backtracking** to perform an exhaustive search.

Backtracking is 'trial-and-error': making decisions until it is clear that a solution is not possible, then undoing previous decisions, to try another route to reach a solution.

Unbounded means that we cannot fix how far back we may need to undo decisions.

The decisions generate a *tree* and exhaustive search means traversing this tree to visit all the nodes.

Example: Travelling around graphs

Consider graphs (directed or undirected), we can consider various path finding problems, such as:

Hamiltonian cycle (after Sir William Hamilton)

Starting at a node, seek a path which travels around the graph, finishing at the start node and visiting all nodes just once.

Travelling Salesperson

For graphs with distances assigned to edges, seek a minimum length Hamiltonian cycle.

Only known algorithms for both problems are by *unbounded* exhaustive backtracking and are therefore exponential.

Why exponential?

$$C_N = N \times C_{N-1} + a$$

because, in the worst case, we make one of N initial choices (the first node visited) and then have a problem of size N-1, the choice requires a computation of fixed amount a.

The solution is $C_N = O(N!) = O(N^N)$.

Other examples: Knapsack problems, games and puzzles

Given an empty box of fixed dimensions, and a number of blocks of various dimensions:

The task is to choose some of the blocks and arrange them in the box so that they occupy a maximum amount of space i.e. the empty (unused) space is minimized.

Algorithms are by exhaustive search.

Other examples: Games and puzzles

Many games and puzzles have only infeasible algorithms. That is what makes them interesting. Compare noughts-and-crosses, which has a simple algorithm.

For example, the *Polyominos* puzzle:

Given a range of pieces, of polyomino shape (ie consisting of squares of constant size fixed together orthogonally, choose some and fit them onto a chessboard to cover all squares exactly (or on any other fixed shape board).

Complexity theory

Question: Given a computational task, what performance of algorithms can we expect for it?

Two approaches:

- Invent a range of 'good' algorithms.
- Look at the nature of the task and try to determine what range of algorithms can exist.

Example: Matrix multiplication

The standard algorithm for multiplication of two $N \times N$ matrices is (obviously) $O(N^3)$. For a long while, this was believed to be the best possible but...

Strassen's algorithm (1968) is $O(N^{2.81...})!!$ and slightly better ones have been devised since (i.e. slightly smaller exponents).

How good can we get? We simply don't know.

There is an obvious **lower bound** (minimum number of operations) of

$$O(N^2)$$

(because there are N^2 results each needing at least one arithmetic operation).

But what happens between these two?

There is a **computational gap** between known lower bounds and known algorithms.

Example: Sorting

The task of sorting is to rearrange a list (of integers, say) into ascending order.

We shall see later that there are algorithms with worst-case time complexity $O(N \times \log(N))$ for this task.

Moreover this is a *lower bound*: we can show that any general sorting algorithm must be at least $O(N \times \log(N))$.

There is no computational gap.

Famous unsolved problem

The examples of tasks which appear to have only exhaustive search algorithms (travelling salesperson, knapsack etc) are believed to be intrinsically exponential (ie there are no faster algorithms).

This is the essence of the famous

$$P \neq NP$$

conjecture in complexity theory.

(P stands for polynomial - those problems which have polynomial algorithms, and NP stands for non-deterministic polynomial, and is the class of problems including travelling salesperson, knapsack problems etc.)