MU4MA016
Algorithms and Data Structures for Computer Programming

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Schedule 2024 :
Week 1 (Sep. 5th) : Sec. 1
Week 2 (Sep. 12th) : Sec. 2.1 and part of 2.2
Week 3 (Sep. 19th) : End of Sec. 2.2 and Sec. 3.1
Week 4 (Sep. 26th) :

Contents

1 Introduction

The course being entitled **Algorithms** and **Data Structures** for **Computer programming**, in this introductory lecture we will briefly discuss each of these three words, trying to highlight by some simple examples the kind of questions which will interest us in the following.

1.1 Algorithm

The following algorithm was originally described by Euclid in order to find the greatest common divisor (gcd) between two positive integers a and b.

Algorithm 1 Euclid's algorithm (original version)

Require: a, b are positive integers
  function GCD(a, b)
    while $a \neq b$ **do**
      if $a > b$ **then**
        $a \leftarrow a - b$
      else
        $b \leftarrow b - a$
      end if
    end while
    return a
  end function

The above description is called `pseudo code`. It is intended to be read my humans, and it must be unambiguous for humans. Instead, computer programs which we will tackle later, are intended to be read by computers (compilers or interpreters), which implies further restrictions on them (both syntaxic and in terms of the operations available).

Among the properties of algorithms, we will be particularly interested in the following :

- Correctness : that is the least one should ask for, but it needs not be overlooked !
- Complexity : both time and space complexity (to be explained below).
- Ease of implementation : because in the end it will need to be turned into a program.

Correctness

In the case of Euclid's algorithm we could argue along the following lines :

1. After each step of the while loop, a and b remain both positive[1] Indeed they must be different to enter the loop and the smaller is subtracted from the larger.

2. Because of the previous claim, the sum $a + b$ decreases strictly after each step of the loop. In particular, there can be at most finitely many steps of the loop and therefore the algorithm will always terminate.

3. Let c be the actual greatest common divisor of a and b. Then after each step of the loop, c is still a divisor of a and b. Indeed, if a number divides two other numbers, then it also divides their difference. Since the algorithm eventually returns (the modified version of) a, let's call it d, it follows that c divides d.

4. We next claim that d divides (the original values of) a and b. To prove this we argue as above, but backward. First, at the end of the while loop we have $a = b = d$, and therefore d divides both a and b. Now if d divides a and b after some (arbitrary) step of the loop, it also did at the previous one. This is because if a number divides two other numbers, it also divides their sum (and running a step backward correspond to changing one of them to the sum of the two).

5. In summary, we have shown on one hand that c divides d (in particular $c \leq d$), and on the other hand that d divides a and b. By definition of c being the greatest common divisor of a and b, it follows that $c = d$, which proves the correctness.

In many cases, proving algorithm correctness proceeds by showing that some form of invariant is preserved during the process (especially when some loops are involved). In the example above, the invariant was the divisibility by c.

Complexity

As mentioned already, for all the algorithms we will study, we shall discuss both **time complexity** and **space complexity**. These notions only make rigorous sense within a so-called *computation* and a *memory* model, but in short :

- The time complexity measures how much computations the algorithm needs to perform in order to provide its result. Since the number may depend on the input values, it is often useful to distinguish between the worst case scenario and some form of average case.

- The space complexity measures the amount of local storage required by the algorithm in order to perform its computations, in addition to the storage of its inputs.

[1]Note to french speaking students : in mathematical english **positive** means "strictement positif"; the french "positif" is instead translated as **non negative**.

In practice the two notions often pull in opposite directions, and the optimum is a matter of compromise.

In the case of Euclid's algorithm, space complexity is trivial: no temporaries are required since only updates of the original variables occur. Time complexity (assuming that comparison and arithmetic operations can all be performed in $O(1)$ time[2]) can easily be computed to be $O(\max(a, b))$, where the worst case happens when one of the two values, say b, is 1 (just think of the routing of the algorithm in that case, leading to a being decreased by 1 at each step until it reaches 1).

The following variant is actually often called the Euclid algorithm too, although it was not presented by Euclid in this form.

Algorithm 2 Euclid's algorithm (improved version)

Require: a, b are positive integers
Require: c a temporary storage for an integer
  function GCD(a, b)
    while $b \neq 0$ **do**
      $c \leftarrow b$
      $b \leftarrow a$ modulo b
      $a \leftarrow c$
    end while
    return a
  end function

Exercise :

- Prove the correctness of this second version.
- Prove that its time complexity is $O(\log(\max(a, b)))$.
  Hint: proceed backward and compare the current values of a and b to the Fibonacci sequence defined by $F_0 = 0$, $F_1 = 1$ *and* $F_{k+2} = F_{k+1} + F_k$.

In practical applications, a logarithmic complexity is a really strong and desirable one, in comparison e.g. here to the linear complexity of the original version. Even worse would be a quadratic, cubic, general polynomial or even non polynomial (abbr. as NP) complexity.

1.2 Data Structure

Consider the following two variants of the birthday-matching problem (i.e. determine if at least two among a class of students have the same anniversary date, omitting year).

[2]As reasonable as it may look, in practice most implementations would implicitly require that the input integers fit in some range allowing them to be represented easily on the architecture, e.g. over 64bits, which by nature kills the whole meaning of $O()$ analysis, but that is what it is...

Algorithm 3 Birthday match using sets

Require: As input, a set of students, called *class*
Require: As temporary storage, a set of students called *visited*

```
Initialize visited as the empty set
for all student a in class do
    for all student b in visited do
        if birthday_match(a, b) then
            return true
        end if
    end for
    Insert a into visited
end for
return false
```

We have implicitly assumed here that we have a notion of *Set*, over which we can *Iterate*, and which we can grow by making use of some *Insert*.

An **Abstract Data Structure (ADS)** is an abstract description of

1. What kind of data can be stored (possibly referring to other existing ADS)
2. What operations can be performed on these data

In terms of time complexity, in worst case scenarios we will need to apply $O(N^2)$ (where N is the number of students in class) times the birthday match check. We should also take into account the time complexity associated to the *Iterate* (for all) and *Insert* functions. These later must either be postulated (as we did for the arithmetic operations in Euclid's), or guaranteed by some implementation of a Concrete Data Structure within a computing and memory model.

In terms of space complexity, the set *visited* may grow at most to a size of N. With the same caution as above regarding theory vs implementation, we will say that the space complexity is therefore $O(N)$.

Note that whenever $N > 365$, the algorithm could exit early with *true*, by an immediate application of the pigeon-hole principle[3] Not only this underlines the caution that should always accompany asymptotic analysis in finite frameworks, but it also suggests a very different variant :

[3]If there are more pigeons than cages, at least two pigeons must share the same cage. In french: "Principe des tiroirs".

Algorithm 4 Birthday match using an array

Require: As input, a set of students, called *class*
Require: As temporary storage, an array A of 365 boolean
  Initialize all entries of A with false
  for all student s in *class* **do**
    Let k be the anniversary date of s (view as an integer $1 \leq k \leq 365$)
    if $A[k] = true$ **then**
      return true
    else
      $A[k] \leftarrow true$
    end if
  end for
  Return false

The time complexity of this variant is now only $O(N)$ (with the same caution as before), and the space complexity is fixed, independently of the size of the class, therefore $O(1)$.

Exercise : Replace 365 by an integer M (imagine we compare some ID numbers instead of birthdays), and assume that both M and N get large but also that $M \gg N$ (by this we mean that M is much larger than N) and that a spatial complexity of $O(M)$ is forbidden because it would be too large in practice. Are we forced to resort to the first version of the algorithm, or could we do better ? (*Hint: hash tables and sorted trees are both in the menu for later*).

The data structures that we shall go over in this course include : arrays, stacks, queues, lists, hash tables, (binary search) trees, heaps and graphs. Different implementations may use different concrete data structures to represent the same abstract data structure. The abstract notion of Set or of Dictionary, is often implemented either via a hash table, or with some form of tree.

1.3 Computer Programming

We are not going to study computer programming per se[4], but we are going to study how to efficiently implement (good) algorithms on computers, using specific languages.

As scientific programmers, there are essentially two choices, which differ by their strong points and limitations.

- Using a high level language, offering a number of high level native data structures, and potentially also an interactive interpreter. This is the case e.g. of Python and its CPython interpreter, or of Julia with its just-in-time (JIT) compiler. This is the easiest to start with, and it can be efficient too when appropriate libraries

[4]In particular this is not a course on the latest hype in C++!

(coded in low level languages) are available for the task of choice, like e.g. Numpy just to name one. This is also a very good test bed for profiling a new algorithm on small data sets, before turning to a lower level language for performance on large scale data sets.

- Using a lower level language, giving a closer access to the hardware or at least to the virtual memory, and which can be compiled into efficient machine code due to compiler optimizations. This is the case e.g. of C/C++, and the one we will use in this course.

The syntax and grammar of C will not be taught in class. There are very good references online, C grammar is easy, and those who have never met with it will catch-up quickly in the first TP classes. From C++(kind of a superset of C) we will only ever borrow a few features that *may* sometimes be handy.

Although lower level languages are said to be closer to the hardware, in this course for the most we will only need to understand an take into account the following. The storage memory is presented to us by the operating system (OS) as a large addressable 1D array, the so-called *virtual memory*, and

1. **The access time needed to bring back some data from RAM to the CPU can be much larger than the typical time needed by the CPU to perform some computation/instruction** (one usually measures time in so-called CPU cycles). As of today, it can be by a factor 100x to 1000x, with respect e.g. to an arithmetic operation.

2. In order to overcome this otherwise huge bottle-neck in computation, a number of physical levels of so-called caches are introduced in between the CPU and the RAM. You can think of these cache levels as smaller but faster access memories, and there are strategies (independent of us) to decide what is kept in cache (I like the analogy of RAM being the university library, the next level of cache is your home bookshelf, and the closest level of cache to CPU is your nightstand). **The important thing to remember as a programmer, is that if some data is put into cache, then the "nearby" data (in the virtual memory 1D array) is brought at the same time, and therefore it will be readily available provided our successive accesses to memory are sufficiently local**.

This notion of *locality* is well understood (and can be experienced!) in the following simple yet typical example of the computation of the product $A * B$ of two matrices, say of size $N \times N$.

Let's first implement it (in language C) in the way you were taught about the matrix product in Math classes. Note first that the memory being a 1D array, matrices need to be "flattened" to be recorded in memory. The so-called *row-major* convention, i.e. line after line, where the equivalent of what we write $A(i, j)$ in math is accessed in $A[i*N+j]$,

is the most popular in C language implementations. The other obvious alternative, the so-called *column-major* convention, was most popular in Fortran language. Which algorithm works best for a matrix product is highly dependent of the choice of the convention, as we shall experience ! In the sequel we choose the *row-major* standard C convention. Note also that in C, indices for array indexing start at *zero*, not at 1 as we usually do in math, this eases address computations.

```
1  void matrix_product1(float C[], const float A[], const float B[], int N)
2  {
3          for (int i = 0; i < N; ++i) {
4                  for (int j = 0; j < N; j++) {
5                          /* Compute C_{i,j} */
6                          C[i * N + j] = 0;
7                          for (int k = 0; k < N; k++) {
8                                  C[i * N + j] += A[i * N + k] * B[k * N + j];
9                          }
10                 }
11         }
12 }
```

When the loop counters i, j or k are incremented, the data locations involved in the actual product computation on line 8 vary differently. An increment of i leads to a jump of N (times the size of a float, not repeated later) in memory for C and A. An increment of k introduces a jump of N in the memory location for B, and finally an increment of j only induces increments of one (i.e. no jump, i.e. local). By far the most problematic of all these is the jump of N introduced by an increment of k : indeed it arises at every of the N^3 steps of the three nested loops. The increment of i causes the same jump of N, but it only occurs N out of the N^3 steps, which is negligible in proportion. This implementation, at least for large values of N, will therefore likely be memory bottlenecked.

Instead, let us propose the following alternative obtained for the most by a permutation of the loops in j and k :

```
1  void matrix_product2(float C[], const float A[], const float B[], int N)
2  {
3          for (int i = 0; i < N; ++i) {
4                  /* Zero initialize C */
5                  for (int j = 0; j < N; j++) {
6                          C[i * N + j] = 0;
7                  }
8                  for (int k = 0; k < N; k++) {
9                          for (int j = 0; j < N; j++) {
10                                 /* Update C_{i,j} */
11                                 C[i * N + j] += A[i * N + k] * B[k * N + j];
```

```
                        }
                }
        }
}
```

Exercise : First convince yourself that this second version also actually computes the product of A and B ! Then analyze the memory accesses as above, and observe that the non local jumps only occur now N^2 out of N^3 times, which is negligible in proportion if N is large, and therefore should better avoid the memory latency problem.

Exercise : Check it in practice by testing e.g. with $N = 1000$, after you will be familiar with C and gcc in the first TP classes. In these tests, try both the compiler optimization `-O0` (i.e. no optimization) and `-O3` (most optimizations).

Proposed solution Here is a proposed test implementation, that will serve for those of you discovering C. Reproduce and test on your own !

data/matrix_multiplication_test.c

```c
#include <stdio.h>      // For printing to the console
#include <stdlib.h>     // For memory allocation (malloc), string to integer
                        // converion (atoi), and generating random numbers (rand)
#include <sys/time.h>   // For implementing a chrono (struct timeval and
#include <time.h>       // For time() function used in random seed generation
                        // gettimeofday). Requires a POSIX OS.

void matrix_product_v1(float *C, const float *A, const float *B, int N) {
        for (int i = 0; i < N; ++i) {
                for (int j = 0; j < N; j++) {
                        C[i * N + j] = 0;
                        for (int k = 0; k < N; k++) {
                                /* Update C_ {i , j } */
                                C[i * N + j] += A[i * N + k] * B[k * N + j];
                        }
                }
        }
}

void matrix_product_v2(float *C, const float *A, const float *B, int N) {
        for (int i = 0; i < N; ++i) {
                /* Zero initialize C */
                for (int j = 0; j < N; j++) {
                        C[i * N + j] = 0;
                }
                for (int k = 0; k < N; k++) {
                        for (int j = 0; j < N; j++) {
                                /* Update C_ {i , j } */
                                C[i * N + j] += A[i * N + k] * B[k * N + j];
                        }
                }
```

```
32          }
33  }
34
35  void timer_start(struct timeval *tv) { gettimeofday(tv, NULL); }
36
37  unsigned int timer_stop(const struct timeval *tv, const char *str) {
38          struct timeval now;
39          gettimeofday(&now, NULL);
40          unsigned int mus = 1000000 * (now.tv_sec - tv->tv_sec);
41          mus += (now.tv_usec - tv->tv_usec);
42          if (str[0]) {
43                  printf("Timer %s: ", str);
44                  if (mus >= 1000000) {
45                          printf("%.3f s\n", (float)mus / 1000000);
46                  } else {
47                          printf("%.3f ms\n", (float)mus / 1000);
48                  }
49          }
50          return (mus);
51  }
52
53  /* When profiling with compiler optimization, it is important to ''do''
54   * something with the result, all of it, in order to prevent the smart
55   * compiler from just no computing what is not latter used.
56   */
57  float check_and_avoid_lazy_optimizers(const float *C, int N) {
58          float dummy = 0;
59          for (int i = 0; i < N * N; ++i) {
60                  dummy += C[i];
61          }
62          return dummy;
63  }
64
65  /* We initialize A and B with random numbers in the interval [0,1] */
66  void initialize_matrices(float *A, float *B, int N) {
67          srand(time(NULL));
68          for (int i = 0; i < N * N; ++i) {
69                  A[i] = (double)rand() / RAND_MAX;
70                  B[i] = (double)rand() / RAND_MAX;
71          }
72  }
73
74  int main(int argc, char **argv) {
75          /* Read 1st program argument string and convert into a number*/
76          int N = atoi(argv[1]);
77          if (N <= 0) {
78                  printf("First argument N must be positive.\n");
79                  return (EXIT_FAILURE);
80          }
81
82          /* Allocate memory for storing A, B, and the resulting C = A * B */
83          float *A = (float *)malloc(N * N * sizeof(float));
```

```
84          float *B = (float *)malloc(N * N * sizeof(float));
85          float *C = (float *)malloc(N * N * sizeof(float));
86          if (A == NULL || B == NULL || C == NULL) {
87                  printf("Memory allocation failed ($N$ too large ?)\n");
88                  return (EXIT_FAILURE);
89          }
90
91          /* For measuring timings of both algorithm */
92          struct timeval chrono;
93
94          /* Test 1 */
95          initialize_matrices(A, B, N);
96          timer_start(&chrono);
97          matrix_product_v1(C, A, B, N);
98          timer_stop(&chrono, "Algo 1");
99          printf("Sum of C : %f\n", check_and_avoid_lazy_optimizers(C, N));
100
101         /* Test 2 */
102         // initialize_matrices(A, B, N);
103         timer_start(&chrono);
104         matrix_product_v2(C, A, B, N);
105         timer_stop(&chrono, "Algo 2");
106         printf("Sum of C : %f\n", check_and_avoid_lazy_optimizers(C, N));
107
108         /* Release memory to OS */
109         free(C);
110         free(B);
111         free(A);
112
113         return (EXIT_SUCCESS);
114 }
```

data/matrix_multiplication_test.c

We then compile it (first with zero optimization) :

```
@: gcc -Wall matrix_multiplication_test.c -o matrix_multiplication_test
```

and test it

```
@: ./matrix_multiplication_test 1000
Timer Algo 1: 4.159 s
Sum of C : 250005104.000000
Timer Algo 2: 3.229 s
Sum of C : 250005104.000000
```

We can observe a modest difference but not great. Let's introduce compiler optimization (level 3 = all).

```
@: gcc -Wall -O3 matrix_multiplication_test.c -o matrix_multiplication_test
@: ./matrix_multiplication_test 1000
Timer Algo 1: 1.031 s
Sum of C : 250005104.000000
Timer Algo 2: 141.192 ms
Sum of C : 250005104.000000
```

First as you can see the -O3 flag implied a great speed-up, but more importantly the `_v2` version of the algorithm also now runs one order of magnitude faster than the `_v1` one !

Remark. Although the matrices A and B were filled with random real numbers between 0 and 1, the sum of the coefficients of C seems to be an integer. How is that possible ?! The (pseudo)-random values stored in A_{ij} and B_{jk} are supposed to model a uniform distribution on $[0, 1]$, therefore

$$\mathbb{E}(sum(C)) = \sum_{i,j,k=1}^{N} \mathbb{E}(A_{ij}B_{jk}) = \sum_{i,j,k=1}^{N} \mathbb{E}(A_{ij})\mathbb{E}(B_{jk}) = \frac{N^3}{4},$$

where we have used that A_{ij} and B_{jk} are independent (they are different samplings of the random variable) and $\mathbb{E}(A_{ij}) = \mathbb{E}(B_{jk}) = \frac{1}{2}$ for a uniform variable over $[0, 1]$. For $N = 1000$, we expect therefore that $\mathbb{E}(sum(C)) = 2.5e8$, which indeed is an integer. But the error itself, in the example sampling above 5104, has no reason to be an integer. This is not at all related to the maths, but instead to the way real numbers (here 32 bits floating points) are stored in a computer, we will discuss that into more details later. Not all real numbers are represented (there would be infinitely many of them!), and it happens that within 32bits floats the closest float to $2.5e8$ is $2.5e8 + 1$. If you take $N = 100$ instead, you'll start observing fractional parts in the answer.

Exercise : Compute that

$$\mathbb{E}(sum(C)^2) = \frac{1}{16}N^6 + \frac{1}{24}N^4 + \frac{1}{36}N^3$$

and therefore that

$$\Sigma(sum(C)) = \sqrt{Var(sum(C))} = \sqrt{N^4/24 + N^3/3} \simeq 0.2N^2 \text{ for N large.}$$

Run the test above multiple times, of with different values of N, and observe/check then that the deviation to the expected value is indeed of the order of the standard deviation $\Sigma(sum(C)) \simeq 0.2N^2$.
Hint : while evaluating terms of the form $\mathbb{E}(A_{ij}B_{jk}A_{i'j'}B_{j'k'})$, distinguish between the three cases : a) $(i, j, k) = (i', j', k')$, b) $(i, j) = (i', j')$ or $(j, k) = (j', k')$ but $(i, j, k) \neq (i', j', k')$, and finally c) $(i, j) \neq (i', j')$ and $(j, k) \neq (j', k')$. Recall also that whenever X is uniform over $[0, 1]$, $\mathbb{E}(X^2) = \int_0^1 x^2\, dx = \frac{1}{3}$.

Finally, let us compare our code performance with respect to Python, either using pure Python loops or using available scientific libraries, the most famous being Numpy (it is internally coded in C!).

data/matrix_multiplication_test.py

```
1 import numpy
2 import time
```

```
3
4  for N in (10, 20, 50, 100, 200):
5
6      A = numpy.random.random((N, N)).astype(numpy.float32)
7      B = numpy.random.random((N, N)).astype(numpy.float32)
8      C = numpy.zeros((N,N)).astype(numpy.float32)
9
10     if (N <= 200):
11         start = time.time()
12         for i in range(N):
13             for k in range(N):
14                 for j in range(N):
15                     C[i,j] += A[i,k] * B[k,j]
16         end = time.time()
17         print("Pure Python for N = %4d : %.5fs" % (N, end - start))
18
19 for N in (1000, 2000, 4000):
20
21     A = numpy.random.random((N, N)).astype(numpy.float32)
22     B = numpy.random.random((N, N)).astype(numpy.float32)
23     C = numpy.zeros((N,N)).astype(numpy.float32)
24
25     start = time.time()
26     tests = int(10000 / N) + 1
27     for i in range(tests):
28         C = A.dot(B)
29     end = time.time()
30     print("Using Numpy for N = %4d : %.5fs" % (N, (end - start) / tests))
```

data/matrix_multiplication_test.py

We obtain :

```
@: python3 matrix_multiplication_test.py
Pure Python for N =   10 : 0.00117s
Pure Python for N =   20 : 0.00923s
Pure Python for N =   50 : 0.07167s
Pure Python for N =  100 : 0.52314s
Pure Python for N =  200 : 4.19137s
Using Numpy for N = 1000 : 0.00737s
Using Numpy for N = 2000 : 0.04697s
Using Numpy for N = 4000 : 0.35011s
```

A number of remarks are in order :

1. For both algorithm, we can observe the expected behaviour of a cubic time complexity. Note that algorithm with a lower power of N do exist (see e.g. this Wiki link), but they are complex to implement and often come with large pre-factor constants. The most well-known is Strassen's algorithm, at $O(N^{\log_2(7)}) \simeq O(N^{2.8})$, but the present state of the art is $O(N^{2.37})$. Clearly any algorithm must be at least $O(N^2)$ (indeed at least the N^2 entries of C must be filled!), at least for a sequential algorithm, but it is open if one could go as low as $O(N^2)$.

2. There is a **huge** difference between the timings in pure Python and using Numpy, more than three orders of magnitude. As a matter of fact, for pure Python I had to limit N to a smaller value than a few hundreds in order to keep the script run time under control.

3. For $N = 1000$, Numpy is still 20 times faster that our current best implementation in `_v2` !

What can/should we do to improve our code to state of the art performance then ? There are easy improvements :

1. Allow the compiler to use the whole set of CPU instructions for the computer we are running on (this can be an issue if we wish to distribute our program to machines which would not have all this set). The gcc option is `-march = native`. A safer yet usually as effective solution is to require a common vector instruction set, like the MMX or AVX. We shall use the `-mavx` gcc switch.

2. Modify our C code by adding the *restrict* keyword to the output array pointer C of our matrix_product functions. This tells the compiler that the place where we write C does not overlap (one says "aliases with") the one of A and or B, and avoids unnecessary copies.

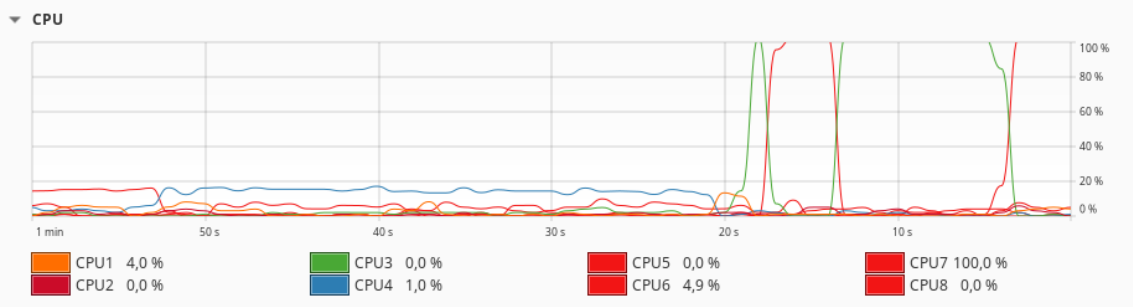
3. Modify our C code by forcing a 256 bits alignment for our memory allocations of A, B and C. This can improve the use of vector instructions by the compiler (see 1) here above). To do so, we replace `malloc` by `aligned_alloc`.

```
1  void matrix_product_v2(float *__restrict C, const float *A,
2                                              const float *B, int N) {
3  [...]
4  }
5
6  [...]
7          float *A = (float *)aligned_malloc(32, N * N * sizeof(float));
8          float *B = (float *)aligned_malloc(32, N * N * sizeof(float));
9          float *C = (float *)aligned_malloc(32, N * N * sizeof(float));
10 [...]
```

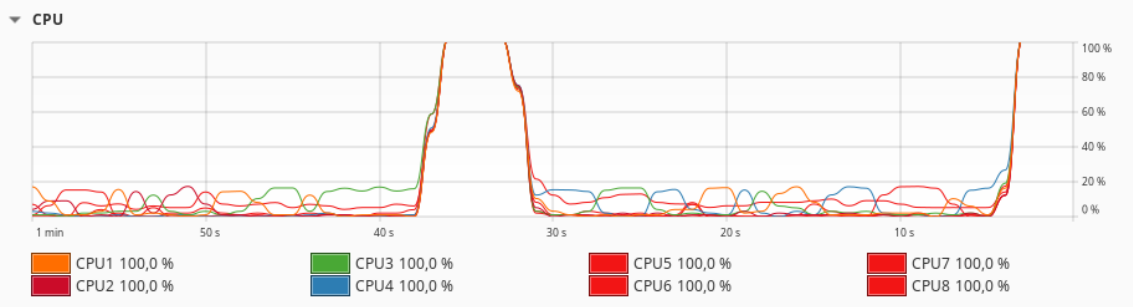
With these and the avx switch we obtain:

```
@: gcc -Wall -O3 -mavx matrix_multiplication_test.c -o
   matrix_multiplication_test
@: ./matrix_multiplication_test 1000
Timer Algo 1: 1.042 s
Sum of C : 250279296.000000
Timer Algo 2: 69.523 ms
Sum of C : 250279296.000000
```

We have improved from $140ms$ to $70ms$, that is a factor 2, not bad ! Be we are still missing a factor almost 10. Let us observe the Operating System Monitor, first during our own implementation :



and then during Numpy's implementation[5]



The road-map is clear : our code is sequential, it uses just one CPU core, while Numpy is making use of parallelism to use all the available 4 cores / 8 threads in my (modest) computer !

Numpy's (quite complex) source code can be browsed on Github here. One C source file for (one of the possible versions of) matrix multiplication is this one. It has many includes and internal preprocessor macros making it difficult to read though, you may even have difficulties to recognize a valid C code.

Turning our matrix multiplication code into a parallel algorithm is one of the very nice projects that you could implement for this course, especially for those of you that are in the HPC program. Either making use of CPU parallelism (using e.g. `OpenMP` or better the lower level `pthread`), or even going to the GPU if one is available on your computer (using e.g. `OpenCL`, `OpenGL/Vulkan` compute shaders, or the proprietary `CUDA`).

In a broader perspective, parallelization of algorithms in many different areas of Math/CS has been a very hot topic in recent years. This yields challenges both at the algorithmic level, and at the implementation level. They require specific courses and we shall not dive too deeply into it, yet they all build upon the concepts we shall develop in this course.

[5]In both cases, we have increased N so has to have time to take a screenshot !

2 Some programming concepts

2.1 Interface vs Implementation

It is always useful and also often important to separate what we will call the *interface* from what we will call the *implementation*. In the table below I have listed a number of concepts : all the ones in the left column correspond (and may be more or less understood as equivalent between each other) to the interface, while all the ones in the right column correspond to the implementation.

On the user side :	On the programmer side :
• Abstract Data Structure	• Concrete Data Structure
• Interface / Documentation	• Implementation
• Application Programming Interface (API)	• Source code
• Header files In C/C++, typically `.h` or `.hpp`	• Source files In C/C++, typically `.c` or `.cpp`

In vague terms the interface *should* :

- describe what kind of data it is designed to handle
- describe what actions on this data it can perform
- possibly offer some guarantee about algorithmic complexity of some of these actions (worst case, expected mean, etc).

It should *not* describe *how* these are implemented. One of the reasons for the latter is the ability to update/improve the implementation without breaking user code.

A key point to have in mind when designing interfaces and implementations is that less methods/actions available in the interface implies :

- less flexibility for the user
- less constraints for the implementation, and therefore possibly better performance

As a rule of thumb : one should not devise overcomplicated data structures, but choose the simplest one(s) that fit all the identified requirements for a task, but no more. Some people call it the KISS philosophy : Keep It Straight and Simple.

An example in the standard C library which one encounters in the very first steps of learning the language is the `FILE` abstract data structure for file IO (i.e. reading and writing to files).

Some typical code would look like

```c
#include <stdio.h>

// [some code here]

FILE *f;
f = fopen("example.txt", "r");
if (f == NULL) {
        // [produce error message and exit]
}

// [do something with f]

fclose(f);
```

What exactly is contained in `FILE` needs not be known to us[6], we shall use it only as a *opaque handle*. In the *header* file `stdio.h` we can find[7] (among other things) the **declaration** :

```c
FILE *fopen(const char *__filename, const char *__modes);
```

which teaches us that the function `fopen` :

- requires two arguments, both of which being of type `char *` (used to represent character strings) and which won't be modified by the function itself (because they are marked with the keyword `const`).
- returns a pointer to a `FILE` data structure.

Most of the time, to access documentation for standard libraries you will instead refer to online documents, like e.g. `https://cplusplus.com/reference/cstdio/fopen/` in the above case.

Whenever we need to do something with the file, we must use the handle (it is called `f` is the sample code above) and pass it to the relevant function, as in :

```c
// [do something with f]
char line[80];
fread(line, 80, f);
```

[6] It is actually a macro for a (complicated) C struct defined in stdio.c

[7] On Linux systems this file is found in `/usr/include/stdio.h`

2.2 Pointer based vs Array based implementation

The implementation of data structures can usually be divided into two families :

1. Array based
2. Pointer based

The difference between both amounts to the way the data is stored in virtual memory.

When array based, the data is stored in a *contiguous* way and it is assumed that each element of the array occupies the same amount of space in memory. The main implication of this is that to recover the element of index `k`, it suffices to fetch memory at the address being computed as the address of the start of the array plus `k` times the size of an array element. In other words, only the address of the start of the array needs to be recorded.

When pointer based instead, the data may be spread across memory. The implication is that each element of the data should be accompanied with a way to access the next and or the previous one(s), typically by storing its/their address(es).

We can therefore quickly foresee the advantages and limitations of both :

- Array based are potentially much faster because they allow for direct access to any element by its index and need not store addresses. On the other hand, the contiguity assumption has some implications on some operations (e.g. suppressing an element would imply a potentially large copy in order to avoid creating a gap, and the same would apply to some insertion in the middle). The question of how large the reserved memory chunk to store the array should be chose is also an important question, especially when it is not known a priori how large the data structure will be eventually (imagine we read elements from a file, and we only know we are finished when we reach its end).

- Pointer based have the exact opposite advantages and limitations. Adding and/or suppressing elements is conceptually and practically simpler, because it only implies modifying a couple of pointers, but that may come at the price of performance. Besides, direct access to the k-th element (whenever it makes sense, not all structures have a natural mapping to sequences, think e.g. of arbitrary trees) is typically not possible for them.

To provide an example of both, and having the goal of separation interface/implementation in mind, in the sequel we propose one common interface and two possible implementations for a *Stack* data structure. This is one of the simplest data structures, and it will therefore serve well our expository purposes. The first implementation will be pointer based, while the second will be array based. User code should should equally work in both cases, as a matter of fact there is nothing in the interface suggesting how it is implemented.

First the interface :

data/stack.h

```c
// A Header file for a Stack of integers API
#include <stdbool.h> /* For bool type   */
#include <stddef.h> /* For size_t type */

struct Stack; /* Declaration only of the type : struct Stack*/
typedef struct Stack Stack; /* Alias :
                             * Allows to write Stack instead of struct Stack */

/* Create a new stack */
Stack *stack_init();

/* Pushes a new element (int) on top of the stack */
void stack_push(Stack *s, int value);

/* Pop the top element from the stack */
/* NOTE : stack should NOT be empty   */
int stack_pop(Stack *s);

/* Dispose an existing stack */
void stack_dispose(Stack *s);

/* Check if stack is empty */
bool stack_is_empty(Stack *s);

/* Number of elements in the stack */
size_t stack_size(Stack *s);
```

data/stack.h

Next the pointer based implementation :

data/stack_pointer_based.c

```c
// A source file for a pointer based implementation of a Stack of integers
#include <stdbool.h>
#include <stddef.h>
#include <stdlib.h>
#include <assert.h>

#include "data/stack.h"

struct StackNode { /* Declaration and Definition of a struct StackNode */
        struct StackNode *next;
        int value;
};
typedef struct StackNode StackNode;

struct Stack { /* Definition of struct Stack */
        struct StackNode *head;
        size_t size;
};

```

```
20 Stack *stack_init()
21 {
22         Stack *s = malloc(sizeof(Stack));
23         if (s != NULL) {
24                 s->head = NULL;
25                 s->size = 0;
26         }
27         return (s);
28 }
29
30 void stack_push(Stack *s, int value)
31 {
32         assert(s != NULL);
33         StackNode *new_node = malloc(sizeof(StackNode));
34         if (new_node == NULL) {
35                 /* Fail silently */
36                 return;
37         }
38         new_node->next = s->head;
39         new_node->value = value;
40         s->head = new_node;
41         s->size++;
42 }
43
44 int stack_pop(Stack *s)
45 {
46         assert(s != NULL && s->size != 0);
47         int res = s->head->value;
48         StackNode *next_head = s->head->next;
49         free(s->head);
50         s->head = next_head;
51         s->size--;
52
53         return (res);
54 }
55
56 void stack_dispose(Stack *s)
57 {
58         if (s == NULL) {
59                 return;
60         }
61         /* First free stack nodes if any */
62         while (s->head != NULL) {
63                 StackNode *old_head = s->head;
64                 s->head = s->head->next;
65                 free(old_head);
66         }
67         /* Then free s itself */
68         free(s);
69 }
70
71 bool stack_is_empty(Stack *s)
```

```
72 {
73         assert(s != NULL);
74         return (s->size == 0);
75 }
76
77 size_t stack_size(Stack *s)
78 {
79         assert(s != NULL);
80         return (s->size);
81 }
```

data/stack_pointer_based.c

And finally the array based one :

data/stack_array_based.c

```
1  // A source file for an array based implementation of a Stack of integers
2  #include <stdbool.h>
3  #include <stdlib.h>
4  #include <assert.h>
5
6  #include "data/stack.h"
7
8  struct Stack { /* Definition of struct Stack */
9          size_t size; /* Number of elements in the stack        */
10         size_t capacity; /* Capacity of the array holding elements */
11         int *data; /* The data array itself                  */
12 };
13
14 Stack *stack_init()
15 {
16         Stack *s = malloc(sizeof(Stack));
17         if (s != NULL) {
18                 s->size = 0;
19                 s->capacity = 0;
20                 s->data = NULL;
21         }
22         return (s);
23 }
24
25 void stack_push(Stack *s, int value)
26 {
27         assert(s != NULL);
28         if (s->size >= s->capacity) {
29                 size_t new_cap = s->capacity == 0 ? 1 : 2 * s->capacity;
30                 int *new_data = realloc(s->data, new_cap * sizeof(int));
31                 if (new_data != NULL) {
32                         s->data = new_data;
33                         s->capacity = new_cap;
34                 } else {
35                         return;
36                 }
```

```
37          }
38          s->data[s->size] = value;
39          s->size++;
40  }
41
42  int stack_pop(Stack *s)
43  {
44          assert(s != NULL && s->size > 0);
45          s->size--;
46          return (s->data[s->size]);
47  }
48
49  void stack_dispose(Stack *s)
50  {
51          if (s == NULL) {
52                  return;
53          }
54          free(s->data);
55          free(s);
56  }
57
58  bool stack_is_empty(Stack *s)
59  {
60          assert(s != NULL);
61          return (s->size == 0);
62  }
63
64  size_t stack_size(Stack *s)
65  {
66          assert(s != NULL);
67          return (s->size);
68  }
```

data/stack_array_based.c

Exercise : Assuming the cost of a memory allocation for a block of size M is $O(M)$, compute that using the doubling strategy for the array capacity in the previous implementation, the average cost for N successive pushes to the stack is only $O(1)$. Instead, realize that any strategy which would be based on a fixed additive capacity increase (rather than a multiplicative strategy) would lead to an $O(N)$ average cost. The factor 2 is not important though, any (possibly non integer) number $r > 1$ would accomplish the same goal.

2.3 Inlining

This subsection can be skipped at first reading, and is mostly meant for students that already have a compiled languages background.

In some cases, a clear separation between the interface and the implementation implies some performance costs which are undesirable. This situation arises when some

utility functions which are implemented are so small and used so often that the function calls themselves end-up accounting for most of the total cost.

To avoid these situations, it is sometimes therefore advisable to *not* separate both the interface and the implementation, so that the compilers will always view the whole code of the given functions when including them elsewhere, and will be able to optimize it better.

As a typical example, the next listing proposes an implementation for an array data structure. It is very much similar to the above array based implementation of a stack data structure, but promoted to an array data structure by adding random access to any index in the array. This is also the occasion to introduce some C++that wouldn't compile as C code : it uses *templates*, and *methods* (in particular constructors and destructors). Both concepts are not present (at least as such) in plain C. They are mostly conveniences for the programmer, and they should be approached with care : do not over-abuse templates if you wish your code to compile fast, and pay attention to unnecessary copies in constructors it you wish your code to run fast !

data/array.hpp

```
1  #pragma once
2
3  #include <assert.h>
4  #include <stdlib.h>
5
6  #define ARRAY_FIRST_CAPACITY 8
7
8  template <typename T>
9  struct TArray {
10         /**
11          * Members
12          */
13         size_t size;
14         size_t capacity;
15         T *data;
16         /**
17          * Methods
18          */
19         TArray();
20         TArray(size_t size);
21         ~TArray();
22         T &operator[](size_t i);
23         const T &operator[](size_t i) const;
24         void push_back(const T &t);
25         T *pop_back();
26         void resize(size_t size);
27         void reserve(size_t capacity);
28         void clear();
29 };
30
31 template <typename T>
```

```
32 TArray<T>::TArray() : size{0}, capacity{0}, data{nullptr}
33 {
34 }
35
36 template <typename T>
37 TArray<T>::TArray(size_t size) : size{size}, capacity{size}
38 {
39         data = static_cast<T *>(malloc(size * sizeof(T)));
40 };
41
42 template <typename T>
43 inline TArray<T>::~TArray()
44 {
45         size = 0;
46         capacity = 0;
47         free(data);
48         data = nullptr;
49 }
50
51 template <typename T>
52 inline T &TArray<T>::operator[](size_t i)
53 {
54         assert(i < size);
55         return (data[i]);
56 }
57
58 template <typename T>
59 inline const T &TArray<T>::operator[](size_t i) const
60 {
61         assert(i < size);
62         return (data[i]);
63 }
64
65 template <typename T>
66 inline void TArray<T>::push_back(const T &t)
67 {
68         if (size >= capacity) {
69                 capacity = capacity < ARRAY_FIRST_CAPACITY
70                                 ? ARRAY_FIRST_CAPACITY
71                                 : 2 * capacity;
72                 data = static_cast<T *>(realloc(data, capacity * sizeof(T)));
73         }
74         data[size++] = t;
75 }
76
77 template <typename T>
78 inline T *TArray<T>::pop_back()
79 {
80         T *ret = NULL;
81         if (size) {
82                 ret = &data[--size];
83         }
```

```
84          return ret;
85  }
86
87  template <typename T>
88  void TArray<T>::resize(size_t size)
89  {
90          this->size = size;
91
92          if (size > capacity) {
93                  data = static_cast<T *>(realloc(data, size * sizeof(T)));
94                  capacity = size;
95          }
96  }
97
98  template <typename T>
99  void TArray<T>::reserve(size_t capacity)
100 {
101         if (capacity > this->capacity) {
102                 data = static_cast<T *>(realloc(data, capacity * sizeof(T)));
103                 this->capacity = capacity;
104         }
105 }
106
107 template <typename T>
108 inline void TArray<T>::clear()
109 {
110         size = 0;
111 }
```

data/array.hpp

If you are familiar with C++, that may remind you of the `std::vector` data structure from the Standard Templated Library (STL). Pay attention though that the `TArray` version above is only really meant for types T that are POD (Plain Old Data), i.e. types that can simply be bitwise copied and in particular have no need for constructors or destructors. In scientific computing the latter are more important and more frequent for the "real data".

We shall now discus the problem of **Searching** in a data structure, i.e. looking for some data based on its *value*.

To make Searching efficient, data structures rely mostly on one or the other of the following two key ideas :

- Sorting
- Hashing

In Section 3 we begin by discussing sorting, in the simple case of arrays, and how it improves searching by e.g. the binary search. In Section 4 we will discuss hashing, and the important related data structure the hash table. Further along we will go back to the question of sorting when discussing data structures which implement sorting while not not being (necessarily) arrays, like (self balancing) binary search trees in section 5.2 and 5.3.

3 Sorting

If an array of size N isn't sorted, the average number of comparisons needed when searching for some data in the array is clearly $O(N)$.

If the array is known to be sorted (say in increasing order), we can improve the search time complexity by relying on the following binary search strategy (*recherche dichotomique* in french).

```
1  // @size : number of elements in the array
2  // @value : value which is searched for
3  float *binary_search(const float *array, size_t size, float value)
4  {
5          size_t begin = 0;
6          size_t end = size - 1;
7
8          while (begin <= end) {
9                  size_t pos = (begin + end) / 2;
10                 if (array[pos] == value) {
11                         return (&array[pos]);
12                 } else if (array[pos] <= value) {
13                         begin = pos + 1;
14                 } else {
15                         end = pos - 1;
16                 }
17         }
18         /* If we reach here value is not present in the array */
19         return NULL;
20 }
```

At each step in the while loop the length of the search interval is divided by two (up to one due do integer division) until the value is found of the size of the search interval drops down to nothing. In particular, their will be at most $O(\log_2(N))$ such steps.

Note that the float type could be replaced by an arbitrary type T (like a user defined struct) provided the latter implements and equality and comparison operators :

```
1  // T should be an existing type, implementing 'is_equal'
2  // and 'is_smaller'.
3  T *binary_search(const T *array, size_t size, T value)
4  {
5          size_t begin = 0;
6          size_t end = size - 1;
7
8          while (begin <= end) {
9                  size_t pos = (begin + end) / 2;
10                 if (is_equal(array[pos], value)) {
11                         return (&array[pos]);
12                 } else if (is_smaller(array[pos], value)) {
13                         begin = pos;
14                 } else {
15                         end = pos;
16                 }
17         }
18         return NULL;
19 }
```

Pay attention that for the previous to work, the comparison function `is_smaller` should implement an order and not just a pre-order on T. This remark is important because in computer science it is common to use pre-orders. These often have the form of an actual order, but acting only on part of the instances of the given type (typically a classical arithmetic compare on one distinct field of a struct - think e.g. of 2D points being ranked according to their x coordinates). If the anti-symmetry property (that is a is smaller than b and b is smaller than a implies that a is equal to b) is not satisfied, then the above algorithm may pick the wrong left or right side in such situations, and therefore would be buggy. Most sorting algorithms are relevant and perfectly work in the case of pre-orders though, the reason why we mention it.

We will next discuss three sorting algorithms. They have been chosen because of both their theoretical and practical importances.

3.1 Insertion sort

Insertion sort is one among if not the fastest sorting algorithm for small arrays. It used also in best in class implementations for large arrays, but in combination with other methods then (e.g. in the later merge sort when the array chunk size decreases below

some predetermined value). It is also of theoretical value because it is one of the few cases where an average time complexity can be rigorously derived without too much pain. At $O(N^2)$, that complexity explains why it can be used alone for large values of N.

The algorithm can be described as follows : at iteration number i the first i elements of the array have already been shuffled between themselves so that they are in order. The $i^{th}+1$ element is then simply moved towards the start of the array as long as it is in wrong order with respect to its predecessor. The latter is achieved by a (possibly empty) sequence of swaps. The fact that the algorithm is in-place (which means that the array is sorted directly with no need of a prior copy or equivalent, that is in $O(1)$ spatial complexity) and that it only uses swaps which by nature are memory cache friendly, explains its speed for small inputs.

```
1  // Sort in increasing order
2  void insertion_sort(float *A, int size)
3  {
4          for (int i = 1; i < size; ++i) {
5                  int j = i;
6                  while (j > 0 && A[j] < A[j-1]) {
7                          float tmp = A[j];
8                          A[j] = A[j - 1];
9                          A[j - 1] = tmp;
10                         j--;
11                 }
12         }
13 }
```

Before we compute the time complexity for a general input array, let us make the following simple observation :

- If the original array A is already in order, then only one comparison (and no swap) will happen at each step of the outer loop. This makes yields a $O(N)$ time cost in such a case, and this is clearly the best case scenario.
- If instead A is initially in reversed order, then each element will need to be swapped with its predecessor until it reaches the start of the array, and therefore the total number of swap will be $\sum_{i=1}^{N-1} i = N(N-1)/2 = O(N^2)$. This is clearly the worst case scenario.

We next show that the average complexity is no better (up to a factor one half) than the worst case. For that purpose, we must first be a little more precise about what we mean be average, i.e. what is the test set over which we will take the average. Assuming for simplicity that all the values in A are distinct (the computation turns out more complicated if not), we simply choose for the test set the one of all possible

permutations of the inputs. We call that set Ω (it satisfies $card(\Omega) = N!$ where N is the number of elements in the array) and we endow it with the uniform probability measure (so that the probability of each input is $1/(N!)$). This is the probability space over which we are going to compute the average cost. More precisely, we are interested in the expectation of the real random variable $C : \Omega \to \mathbb{R}$ which to each input array in Ω associates the number of swaps performed by insertion sort on that input.

The computation of C doesn't seem straightforward at first. Let us say that the elements at position i and j in the array are inverted if $i < j$ but $A[i] > A[j]$. An array is therefore sorted if an only if if does not contain any inversion. The key observation is that because insertion sort only swaps elements which are consecutive in the array (we mean consecutive in terms of their positions in the array, not their values!) each swap resolves one and only one inversion (the one involved in the swap). It follows that the total cost C is exactly equal to the total number of inversion in the input. In mathematical terms :

$$C = \sum_{i<j} I_{i,j},$$

where $I_{i,j}$ is the random (Bernoulli) variable which is one if elements in positions i and j are inverted and zero if not.
The variables $I_{i,j}$ are not independent between themselves, but expectation is a linear feature which does not requires independence. Hence

$$\mathbb{E}(C) = \sum_{i<j} \mathbb{E}(I_{i,j}).$$

The expectation of $I_{i,j}$ (for whatever $i < j$) can easily be seen to be exactly equal to $1/2$. Indeed, there are exactly half of the permutations in Ω for which the i^{th} and j^{th} are in order, and the other half for which they are in reversed order (the permutation of both elements is a bijection between these two sets). It follows that

$$\mathbb{E}(C) = \sum_{i<j} \frac{1}{2} = \frac{N(N+1)}{4}.$$

In summary

1. Worst and average time complexity $O(N^2)$.
2. Time complexity $O(N)$ is the array is already sorted (or "close" to being so).
3. Space complexity reduced to a minimum, the algorithm is in-place.

Note that the algorithm is also stable : this means that the relative position order within the array between elements that are equal in value is not changed between the input and the output. This can be of particular interest when sorting according to a pre-order.

3.2 Merge sort

The merge sort algorithm is a nice and simple example of a *divide and conquer* strategy. To sort an array of size N, it suffices to sort separately the two halves of it, and then to merge the resulting sorted halves into one fully sorted array. The sorting of each of the two halves can be obtained following the same strategy, giving the whole process a recursive nature.

Let's analyze firs the merge part. The following routine merges two arrays A of size sA and B of size sB, supposedly both already sorted, into an array C (of size $sA+sB$).

```
1  void merge(const float *A, int sA, const float *B, int sB, float *C)
2  {
3          int idxA = 0;
4          int idxB = 0;
5          for (int idxC = 0; idxC < sA + sB; idxC++) {
6                  /* if A has not been emptied yet and either B was emptied or
7                   * the tracked element in A is smaller than the one in B,
8                   * we pick from A */
9                  if ((idxA < sA) && ((idxB == sB) || A[idxA] <= B[idxB]))
10                 {
11                         C[idxC] = A[idxA++];
12                 }
13                 /* otherwise we necessarily pick from B */
14                 else
15                 {
16                         C[idxC] = B[idxB++];
17                 }
18         }
19 }
```

Clearly its complexity is $O(sA + sB)$. If we apply the divide and conquer strategy indicated above, and call $T(N)$ the cost of sorting an array of size N is that way, then it follows that

$$T(N) \leq 2 * T(N/2) + cN,$$

for some positive constant c. In case $N = 2^K$, we obtain

$$T(2^K) \leq 2T(2^{K-1}) + c2^k,$$

in which we can again bound $T(2^{K-1})$ similarly and get

$$T(2^K) \leq 2\left(2 * T(2^{K-2}) + c2^{K-1}\right) + c2^K = 2^2T(2^{K-2}) + 2c2^K.$$

Iterating, we finally get down to

$$T(2^K) \leq 2^K T(2^0) + cK2^K.$$

But $T(1) = 0$ (an array of size 1 is already sorted), and $K = \log_2(N)$, therefore

$$T(N) = O(N \log_2(N)).$$

The reasoning extends easily to an arbitrary integer (just pick the smallest power of two larger than N and a monotonicity argument with respect to N). This shows that the time complexity of merge sort is $O(N \log_2(N))$. It can be shown that a sorting algorithm that is based exclusively on comparisons (as merge sort and insertion sort are), cannot do better than this bound. In the next subsection, we will discover a sorting algorithm which is linear in N: it is not based on comparison and imposes some restriction on the data it can sort.

We have not presented a full implementation of the whole merge sort algorithm, only its merge part. In the tutorial class TP1 you will have to bridge that gap. As we shall see (and also transpires from the array C in the merge routine), the process is not done in-place but typically requires one copy of the initial array, leading to a spatial complexity of $O(N)$. In the divide process, it is a good idea to branch to the insertion sort algorithm (rather than a further divide into two) when the size of the array chunk to be sorted falls below a fixed threshold, the optimal value being architecture dependent but probably somewhere in between 8 and 32 (test it!).

3.3 Radix sort

The previous two sorting algorithms which we described were based on comparisons only. For such algorithms, it can be proved that the $O(\log(N))$ complexity achieved my merge sort is optimal.

The sorting algorithm which we describe next is *not* based on comparisons. Instead it relies on counting the number of times the values taken by the elements of the array arise. In a sense this is similar to the solution of the birthday matching problem, which we already discussed, which was based on an array of 365 entries. In that simple variant, the algorithm is called the *counting sort* or sometimes also *bucket sort*:

- Loop over all elements of the array and record the counts for all occurring values
- Accumulate these counts to compute offsets in the final sorted array (the offset for each value is the sum of the counts of all values in the array smaller than itself)
- Loop a second time over all elements of the array and place them directly in correct output position by reading it in the offset array (and incrementing the latter)

Note that by construction this algorithm is $O(N)$ (we do two passes over the data).

Let us illustrate that on birthday sorting :

```c
/* The input array 'unsorted' is assumed to contain N integers all
 * in between 1 and 365.
 * These are sorted in the output array 'sorted' (assumed to be
 * already allocated)
 */
void birthday_counting_sort(int *sorted, const int *unsorted, int N)
{
        int counts[365];
        int offsets[365];

        /* Init counts to zero */
        for (int i = 0; i < 365; i++) {
                counts[i] = 0;
        }

        /* Count occurrences */
        for (int i = 0; i < N; i++) {
                // Shift by one, we have assumed 1st Jan = 1 but
                // C array indices start at 0.
                int bucket = unsorted[i] - 1;
                counts[bucket]++;
        }

        /* Accumulate counts into offsets */
        int offset = 0;
        for (int bucket = 0; bucket < 365; bucket++) {
                offsets[bucket] = offset;
                offset += counts[bucket];
        }

        /* Write back sorted birthdays */
        for (int i = 0; i < N; i++) {
                int bucket = unsorted[i] - 1;
                sorted[offsets[bucket]] = unsorted[i];
                offsets[bucket] += 1;
        }
}
```

The obvious limitation of counting sort is that it is only useful if the number of values potentially taken by the elements of the array is known to be not too large (365 in the previous toy example), at least compared the number of elements to be sorted.

To overcome that limitation, the idea behind *radix sort* is simply to apply counting sort successively on each "digit" of the data, assuming that the data can be described in such a form and that each "digit" can only take a limited number of values (making it appropriate for counting sort).

Imagine for example we need to sort N strings of fixed length k

$$A[i] = c_{1,i}c_{2,i}\cdots c_{k,i},$$

in lexicographical order. Here each $c_{j,i}$ ($1 \leq j \leq k$, $0 \leq i \leq N-1$) belongs to the alphabet set $\{a, b, c, d, \cdots, y, z\}$. We can apply counting sort (with 26 buckets) successively for each positional character, where each output array is used as the input of the next pass of counting sort. That would lead to a cost of $O(kN)$, and if k is considered a fixed constant then this is $O(N)$. But *care must be taken in the order in which be do the successive passes* : we need to start from the last character, and finish with the first one (this is called LSD radix sort for Least Significant Digit). Indeed, if we do it reversely, it is easy to realize that the sort obtained e.g. in the first pass will be destroyed in general by the second (and following) passes. The drawback of this ordering of the counting sort passes is that the Most Significant Digit (here character) only gets considered last, and therefore up until the last pass the array is potentially far from being sorted. A variant of radix sort (called MSD radix sort) applies counting sort starting from the most significant digit. In order to avoid the trap which we discussed above, the second pass is not applied to the full array, but successively to all buckets formed in the first pass (it is usually implemented using recursion). This has the advantage that already after the first pass the array in closer to its final state (this has implication on performance because we know that changes to memory are faster when the corresponding addresses are close to each other, for cache reasons), but on the other hand relying of recursion and having to apply counting sort to all buckets instead of just once potentially counterbalance negatively that advantage.

In the following code listings, we have implemented radix sort for an array of `uint32_t`. These unsigned integers are coded over 32bits :

$$b_{31} \cdots b_0 \mapsto value = \sum_{i=0}^{31} b_i 2^i,$$

where each $b_i \in \{0, 1\}$, leading to a value in the range $\{0, \cdots, 2^{32} - 1\}$.

The granularity (i.e. the choice of the radix/alphabet) is important in practice. We could do 32 passes, one over each bit, but that would be very inefficient (very few work done on each pass). We could also do just one pass with 2^{32} buckets, but that would be both inefficient (lots of zeros in counts) and memory hungry (2^{32} * 4 bytes per int = 16Gb of RAM just for the count array). Instead we shall do it in 4 passes by considering each sequence of 8 bits (i.e. each byte) as a 'digit'. The counting sort will therefore rely on $2^8 = 256$ buckets.

The following optimizations have been made (try to track and understand them in the code) :

- In order to minimize memory allocation/waste, we ping-pong between each pass between the input and the output array (see e.g. in radix_sort_lsd).
- In the MSD implementation, which is recursive, if the number of elements in some bucket becomes too small (we choose 32), instead of pursuing the recursion we switch to insertion sort, which we know is fast if not the fastest for small array size.

- In the second listing, we implement counting sort in place, i.e. with no memory allocation at all and placing the sorted output in place of the input. This requires some care (the key section is the last 'write back' loop on lines 26 to 40 in the function `counting_sort_in_place`)

The code includes a `main` which will allow you to test the timings, and even compare them to the sorting algorithms available in the standard library. You should be convinced afterwards that radix sort is very competitive (tests should use large values of N to be meaningful, like $N = 10^6$ or even 10^7.

```
1  /* NOTE : For comparing performance w.r.t. the standard library we use
2   *        the \cpp std::sort, which has the reputation of being highly optimised.
3   *        This makes our main program dependent on a \cpp compiler, use
4   *        therefore g++ in place of gcc.
5   */
6
7  #include <algorithm>    /* For std::sort
8  #include <stdint.h>     /* For uint32_t type */
9  #include <stdio.h>      /* For printf
10 #include <stdlib.h>     /* For malloc and free */
11 #include <string.h>     /* For memset */
12 #include <time.h>       /* For time to init random nbr generator */
13 void counting_sort(uint32_t *dst, const uint32_t *src, int start, int stop,
14                    int *counts, int *offsets, int bit_shift)
15 {
16         memset(counts, 0, 256 * sizeof(int));
17
18         /* Count occurrences */
19         for (int i = start; i < stop; i++) {
20                 int bucket = (src[i] >> bit_shift) & 0xFF;
21                 counts[bucket]++;
22         }
23
24         /* Accumulate counts into offsets */
25         int offset = start;
26         for (int bucket = 0; bucket < 256; bucket++) {
27                 offsets[bucket] = offset;
28                 offset += counts[bucket];
29         }
30
31         /* Write back (partially) sorted values */
32         for (int i = start; i < stop; i++) {
33                 int bucket = (src[i] >> bit_shift) & 0xFF;
34                 dst[offsets[bucket]++] = src[i];
35         }
36
37         /* Put back offsets to their correct values */
38         for (int bucket = 0; bucket < 256; bucket++) {
39                 offsets[bucket] -= counts[bucket];
```

```
        }
}

void radix_sort_lsd(uint32_t *A, int num)
{

        int counts[256];
        int offsets[256];

        uint32_t *B = (uint32_t *)malloc(num * sizeof(uint32_t));

        counting_sort(B, A, 0, num, counts, offsets, 0);
        counting_sort(A, B, 0, num, counts, offsets, 8);
        counting_sort(B, A, 0, num, counts, offsets, 16);
        counting_sort(A, B, 0, num, counts, offsets, 24);

        free(B);
}

void radix_sort_recursive(uint32_t *dst, uint32_t *src, int start, int stop,
                          int bit_shift)
{
        int counts[256];
        int offsets[256];

        counting_sort(dst, src, start, stop, counts, offsets, bit_shift);

        if (!bit_shift)
                return;

        /* Sort each bucket recursively */
        for (int bucket = 0; bucket < 256; bucket++) {
                if (!counts[bucket])
                        continue;
                int bstart = offsets[bucket];
                int bstop = bstart + counts[bucket];
                if (counts[bucket] <= 32) {
                        /* Switch to insertion sort */
                        /* Need ping-pong in odd passes */
                        uint32_t *final = dst;
                        if (bit_shift != 16) {
                                final = src;
                                memcpy(final + bstart, dst + bstart,
                                       counts[bucket] * sizeof(uint32_t));
                        }
                        for (int i = bstart + 1; i < bstop; i++) {
                                for (int j = i;
                                     j > bstart && final[j] < final[j - 1];
                                     j--) {
                                        uint32_t tmp = final[j];
                                        final[j] = final[j - 1];
                                        final[j - 1] = tmp;
```

```
                                }
                        }
                } else {
                        radix_sort_recursive(src, dst, bstart, bstop,
                                             bit_shift - 8);
                }
        }
}

void radix_sort_msd(uint32_t *A, int num)
{
        uint32_t *B = (uint32_t *)malloc(num * sizeof(uint32_t));
        radix_sort_recursive(B, A, 0, num, 24);
        free(B);
}

void print_array(uint32_t *A, int num)
{
        for (int i = 0; i < num; i++) {
                printf("%d\n", A[i]);
        }
}


int main(int argc, char **argv)
{
        if (argc < 3) {
                printf("Syntax radix_sort n [lsd/msd/stdsort]\n");
        }

        int n = atoi(argv[1]);

        /* Fill a random array */
        uint32_t *A = (uint32_t *)malloc(n * sizeof(uint32_t));
        srand(time(NULL));
        for (int i = 0; i < n; i++) {
                A[i] = rand();
        }

        if (n < 10) {
                printf("Initial array :\n");
                print_array(A, n);
        }

        if (argv[2][0] == 'l') {
                radix_sort_lsd(A, n);
        } else if (argv[2][0] == 'm') {
                radix_sort_msd(A, n);
        } else {
                std::sort(A, A + n);
        }

```

```
144         if (n < 10) {
145                 printf("Sorted array :\n");
146                 print_array(A, n);
147         }
148 
149         return EXIT_SUCCESS;
150 }
```

Next, the version in place, i.e. with no need for a copy of the input array.

```
1  #include <algorithm>
2  #include <stdint.h>
3  #include <stdio.h>
4  #include <stdlib.h>
5  #include <string.h>
6  #include <time.h>
7  
8  void counting_sort_in_place(uint32_t *A, int start, int stop, int *counts,
9                              int *offsets, int *tops, int bit_shift)
10 {
11         memset(counts, 0, 256 * sizeof(int));
12 
13         /* Count occurrences */
14         for (int i = start; i < stop; i++) {
15                 int bucket = (A[i] >> bit_shift) & 0xFF;
16                 counts[bucket]++;
17         }
18 
19         /* Accumulate counts into offsets and tops*/
20         int offset = start;
21         for (int bucket = 0; bucket < 256; bucket++) {
22                 offsets[bucket] = tops[bucket] = offset;
23                 offset += counts[bucket];
24         }
25 
26         /* Write back (partially) sorted values         */
27         /* The effort to do the work in place is here ! */
28         for (int bucket = 0; bucket < 256; bucket++) {
29                 while (tops[bucket] < offsets[bucket] + counts[bucket]) {
30                         int target_bucket =
31                             (A[tops[bucket]] >> bit_shift) & 0xFF;
32                         if (bucket == target_bucket) {
33                                 tops[bucket]++;
34                         } else {
35                                 uint32_t tmp = A[tops[target_bucket]];
36                                 A[tops[target_bucket]++] = A[tops[bucket]];
37                                 A[tops[bucket]] = tmp;
38                         }
39                 }
```

```
        }
}

void radix_sort_lsd_in_place(uint32_t *A, int num)
{
        int counts[256];
        int offsets[256];
        int tops[256];
        counting_sort_in_place(A, 0, num, counts, offsets, tops, 0);
        counting_sort_in_place(A, 0, num, counts, offsets, tops, 8);
        counting_sort_in_place(A, 0, num, counts, offsets, tops, 16);
        counting_sort_in_place(A, 0, num, counts, offsets, tops, 24);
}

void radix_sort_recursive_in_place(uint32_t *A, int start, int stop,
                                   int bit_shift)
{
        int counts[256];
        int offsets[256];
        int tops[256];

        counting_sort_in_place(A, start, stop, counts, offsets, tops,
                               bit_shift);

        if (!bit_shift)
                return;

        /* Sort each bucket recursively */
        for (int bucket = 0; bucket < 256; bucket++) {
                if (!counts[bucket])
                        continue;
                int bstart = offsets[bucket];
                int bstop = bstart + counts[bucket];
                if (counts[bucket] <= 32) {
                        /* Switch to insertion sort */
                        for (int i = bstart + 1; i < bstop; i++) {
                                for (int j = i; j > bstart && A[j] < A[j - 1];
                                     j--) {
                                        uint32_t tmp = A[j];
                                        A[j] = A[j - 1];
                                        A[j - 1] = tmp;
                                }
                        }
                } else {
                        radix_sort_recursive_in_place(A, bstart, bstop,
                                                      bit_shift - 8);
                }
        }
}

void radix_sort_msd_in_place(uint32_t *A, int num)
{
```

```
92          radix_sort_recursive_in_place(A, 0, num, 24);
93  }
94
95  int main(int argc, char **argv)
96  {
97          if (argc < 3) {
98                  printf("Syntax radix_sort_in_place n [lsd/msd/stdsort]\n");
99          }
100
101         int n = atoi(argv[1]);
102
103         /* Fill a random array */
104         uint32_t *A = (uint32_t *)malloc(n * sizeof(uint32_t));
105         srand(time(NULL));
106         for (int i = 0; i < n; i++) {
107                 A[i] = rand();
108         }
109
110         if (argv[2][0] == 'l') {
111                 radix_sort_lsd_in_place(A, n);
112         } else if (argv[2][0] == 'm') {
113                 radix_sort_msd_in_place(A, n);
114         } else {
115                 std::sort(A, A + n);
116         }
117
118         return EXIT_SUCCESS;
119 }
```

At the end of the lecture, we have also discussed the representation of floating point numbers. In particular, we have described the FP32 format of IEEE 754 standard (as followed by the type `float` in C) as well as the FP64 format (followed by the type `double` in C). It is a very good exercise to understand/realize that radix sort (with a slight modification to account for signedness) can be used for these types as well.

4 Hashing

Up to now, when we read N values $a_0, \cdots, a_{N-1}$ of some type T, we stored them in an array A:

$$A[i] = a_i.$$

In functional terms $A : \{0, \cdots, N-1\} \to \mathcal{T}$, where we denote here by $\mathcal{T}$ the set of all elements of type T. In such situation a look-up by index, i.e. $i \mapsto A[i]$, is $O(1)$.
What about a look-up by value ? (i.e. a search/find) :

$$\text{Given } a \in \mathcal{T}, \quad \text{find } i \in \{0, \cdots, N-1\} \text{ s.t. } A[i] = a.$$

We have seen that if A is sorted by some order on $\mathcal{T}$, then binary search can be used to provide an answer in $O(\log(N))$ time. In the general case, we can do no better than linear search which only answers in $O(N)$ time in the mean.

Goal next: When reading the values, insert $a_i \equiv a$ not in position i but in a position $h(a)$ depending (only) on its value a, i.e.

$$A[h(a)] = a.$$

We use the letter h because these functions shall be called *hash* functions. If we can achieve this goal then the look-up by value problem will turn-out to be $O(1)$ (provided, we will come back to it, that evaluation of h is $O(1)$).

Framework: In the sequel we abstract ourselves from the restriction that the values we received came sequentially, instead we shall consider them as a set of so-called *keys*. More precisely, we shall note

- $\mathcal{T}$ the set of all potential keys,
- $\mathcal{K} \subset \mathcal{T}$ the set of actual keys, and we write $N := \#(\mathcal{K})$,
- A an array of size M meant to store keys,
- $h : \mathcal{T} \to \{0, \cdots, M-1\}$ a function.

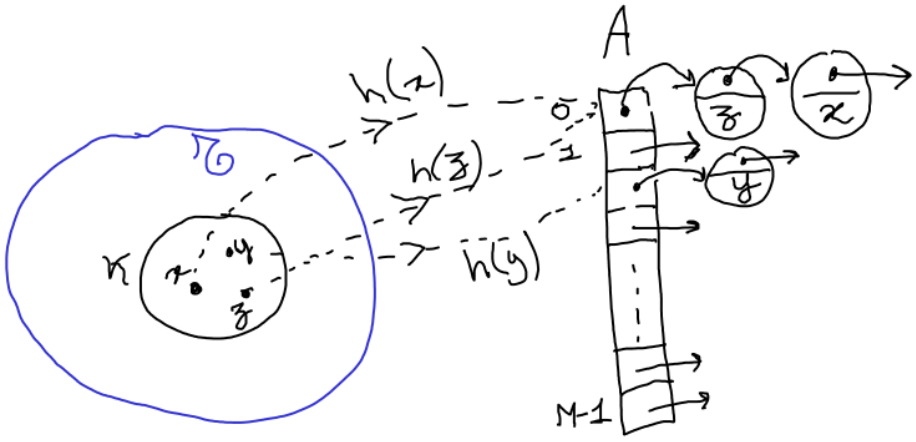
The integers N and M need no longer be equal. We'd like to have

$$\forall\ key \in \mathcal{K},\ \text{set } A[h(key)] = key.$$

Caveat : What if $h(key_1) = h(key_2)$ for some $key_1 \neq key_2 \in \mathcal{K}$?
That situation we shall refer to as a *colliding pair*.
Note that if $N > M$, then by the pigeon-hole principle there must be at least one such pair in $\mathcal{K}$, whatever the hash function h is. Even when $N \leq M$, we shall encounter many situations where in practice it is hopeless to completely avoid colliding pairs.

4.1 Collision work-around # 1 : chaining

The simplest conceptual work-around to collisions is to consider A as an array of linked-list of keys, rather than an array of keys. Whenever a key is hashed into a position that is already occupied, it is simply pushed into the chain there. If the position was instead unoccupied, a chain is initiated with that key.



This work-around is relatively easy to implement *if* we allow ourselves memory allocation on each new insert. It is also the easiest to analyze from a theoretical point of view. In particular,

$$\text{look-up time } = O(\text{length of chain at the corresponding table slot}). \tag{1}$$

Later we will discuss a second work-around, open addressing, that avoids linked lists and allocations on each new insert. It generally leads to better performance in practice, is also easy to implement, but is more complicated to analyze from a theoretical standpoint.

4.2 What is a good hash function ?

We should try to settle the following two questions :

- What is a good hash function ? In view of (1) it should lead to as few collisions as possible (at least for pairs of keys in $\mathcal{K}$, if it is known prior to h, or for pairs of keys in $\mathcal{T}$ otherwise). It should also be fast to evaluate, as we already mentioned.
- What should be M ? If we consider that N is an input (the number of keys we must deal with) and M is a design choice, then certainly we would like that M is not too large with respect to N (anything above N can be considered as "wasted space". Typically, we could be pleased with $M = O(N)$. On the other end of the spectrum there is no minimal requirement if we use chaining, M could be chosen as small as 1, but that would of course have implications on chains lengths and therefore on look-up time. So we should have in mind that M and N should be of the same order.

To make clear the fact that the cost of evaluation of h matters, here is an example of a hash function (assuming $\mathcal{K} = \{a_0, \cdots, a_{M-1}\}$ is known) that leads to zero collision (by construction!) over $\mathcal{K}$), but yet would be a terrible choice :

```
/* T is an arbitrary type
 * a_0, ..., a_{N - 1} are constant literals of type T
 * is_equal implements equality on T x T
 */
int bad_hash(T key)
{
        if (is_equal(key, a_0)) {
                return 0;
        } else if (is_equal(key, a_1)) {
                return 1;
        } else if (is_equal(key, a_2)) {
[...]
[...]
        } else if (is_equal(key, a_{N - 1})) {
                return (N - 1);
        } else {
                /* Don't care for keys out of K */
                return N;
        }
}
```

The elephant in the room is of course that evaluation of *bad_hash* is $O(N)$, which annihilates the whole potential benefit of hashing.

To minimize collisions, we have the intuitive idea that the keys should be spread "evenly" by h. If we must choose h before knowing $\mathcal{K}$ (the most common situation in applications), then we must deal with the following bad news :

Lemma 1. *If $\#(\mathcal{T}) > (N-1)M$ then whatever hash function $h : \mathcal{T} \to 0, \cdots, M-1$ is chosen, there exists an (unlucky) set of keys $\mathcal{K} \subset \mathcal{T}$ such that $\#(\mathcal{K}) = N$ and all keys in $\mathcal{K}$ are hashed by h to the exact same value.*

In other words, there is no universally good hash function if the potential set of keys is too large with respect to the actual set of keys (which, in practice, will be the case almost all the time).

Proof. We may decompose

$$\mathcal{T} = \cup_{i \in \{0, \cdots, M-1\}} h^{-1}(i),$$

where the union is disjoint by construction. In particular

$$\#(\mathcal{T}) = \sum_{i=0}^{M-1} \#(h^{-1}(i)).$$

There must therefore exists at least some $0 \leq i_0 \leq M-1$ for which

$$\#(h^{-1}(i_0)) \geq \frac{\#(\mathcal{T})}{M} > N-1,$$

where we have used the assumption on $\#(\mathcal{T})$ for the last inequality. It suffices then to choose for $\mathcal{K}$ an arbitrary subset of $h^{-1}(i_0)$ of cardinality N. □

4.3 Randomized hash functions and perfect hashing

Although we have just seen that we cannot avoid black swans, we still wish to devise hash functions that will try to efficiently spread keys evenly in the range $0, \cdots M-1$.

It is tempting to use some kind of randomness. Imagine for a second that for each key, $h(key)$ is a random function equally distributed in $0, \cdots, M-1$ and that $h(key_1)$ and $h(key_2)$ are independent whenever $key_1 \neq key_2$. In such situation, we would have for the probability of collisions :

$$\begin{aligned} P\big(h(key_1) = h(key_2)\big) &= P\big(\cup_{i=0}^{M-1} \{h(key_1) = h(key_2) = i\}\big) \\ &= \sum_{i=0}^{M-1} P\big(h(key_1) = h(key_2) = i\big), \end{aligned}$$

and from the independence and uniform distribution assumptions

$$\begin{aligned} \sum_{i=0}^{M-1} P\big(h(key_1) = h(key_2) = i\big) &= \sum_{i=0}^{M-1} P\big(h(key_1) = i\big) P\big(h(key_2) = i\big) \\ &= \sum_{i=0}^{M-1} \frac{1}{M^2} = \frac{1}{M}. \end{aligned}$$

Somehow we deduce from the former analysis that the target we should set ourselves is

$$\forall key_1 \neq key_2 \in \mathcal{T}, P\big(h(key_1) = h(key_2)\big) \leq \frac{1}{M}. \tag{2}$$

The elephant in the room with our previous tentative is that if $h(key)$ uses randomness it is evaluation, then look-ups will be doomed because the evaluation will turn up different at insertion and at look-up time.

Rather than using randomness in the *evaluation* of $h(key)$, we will instead use randomness in the *design* of h (but for similar reasons as just above, we should end up using the same h for all operations after is has been chosen).

In the sequel, we therefore let $\Omega \subset \{0, \cdots, M-1\}^{\mathcal{T}}$ be a set of potential hash functions (note that M is fixed up-front). We also endow Ω with a probability P (in practice, often the uniform probability on Ω). We shall say (Ω, P) is a *universal* family of hash functions precisely when (2) holds.

We have

Lemma 2. *Assume that the hash function h is picked in Ω according to P, and that it is used to fill a hash table of size M using chaining. Assume that this hash table is used for an arbitrary sequence of inserts/deletes/look-up operations which never lead to its total size N growing over $N = cM$, where $c > 0$ is an arbitrary but fixed constant. Then the expectation according to P of the average cost of each of these operations is $O(1)$.*

This result is main theoretical selling point of hash tables, compared to the costs $O(log(N))$ or even $O(N)$ which we discussed earlier. Of course it only holds in expectation, as we have seen that there cannot be a satisfactory a priori guarantee for whatever fixed h.

Proof. We analyze the cost of an insertion, the reasoning for deletions and look-ups are very similar. We know that in the case of chaining the cost of an insertion is proportional to the length of the chain at the corresponding table slot. That number equals the number of keys already in the table at that collide with the inserted key. In expectation, and if the family from which h is picked in universal, that number is $O(N/M) = O(1)$ in view of the assumption $N \leq cM$. □

Remark. Note the subtlety in the above statement that in order for the number of insert / delete / look-up operations to tend to infinity (that's the only framework where $O(1)$ is meaningful) and at the same time verify that $N \leq cM$ (while M is fixed, it must pre-exist Ω), it is necessary that in the sequence of operations deletes compensate inserts in the long run.

Examples of universal families : Assume that the elements $\mathcal{T}$ are fixed size and can be identified with a sequence $b_1 \cdots b_l$ of l chunks each one composed of B bits (and therefore holding a value in the set $0, \cdots, 2^B - 1$). We fix a *prime* integer $M > 2^B$. For each choice of multiplicative coefficients $m_1, \cdots, m_k \in \{0, \cdots M-1\}^k$, we define the hash function

$$h(b_1 \cdots b_l) = \sum_{i=1}^{l} m_i b_i \text{ modulo } M.$$

We pretend that endowed with the uniform probability over $\{0, \cdots M-1\}^k$, this constitutes a universal family of hash functions. Indeed, let $key_1 = b_1 \cdots b_l$ and $key_2 = b'_1 \cdots b'_l$ be distinct. In particular there exists at least one $1 \leq i_0 \leq l$ for which $b_{i_0} \neq b'_{i_0}$. The collision $h(key_1) = h(key_2)$ arises if and only if

$$m_{i_0}\Big(b_{i_0} - b'_{i_0}\Big) = \sum_{i \neq i_0} m_i \Big(b'_i - b_i\Big).$$

Whenever the coefficients m_i with $i \neq i_0$ are chosen, the right hand side above is fixed (let's call it c_{i_0}) and we may rewrite the equation as

$$m_{i_0}\Big(b_{i_0} - b'_{i_0}\Big) = c_{i_0}. \tag{3}$$

By assumption $0 \leq b_{i_0}, b'_{i_0} \leq 2^B - 1 < M$, and $b_{i_0} \neq b'_{i_0}$. In particular $b_{i_0} - b'_{i_0} \neq 0 \bmod M$. Since M is prime (and therefore $\mathbb{Z}/M\mathbb{Z}$ is a finite field), equation (3) possesses one and only one solution $m_{i_0} \in \{0, \cdots, M-1\}$, namely

$$m_{i_0} = \Big(b_{i_0} - b'_{i_0}\Big)^{-1} c_{i_0} \mod M,$$

where the inverse is intended for multiplication modulo M. Since m_{i_0} is chosen according to the uniform probability over $0, \cdots, M-1$, it follows that

$$P\Big(h(key_1) = h(key_2)\Big) = \frac{1}{M}.$$

This shows that the family is universal.

In the same spirit as for Lemma 2, and with essentially the same proof, we have

Lemma 3. *Let M be fixed, (Ω, P) we a universal family of hash functions, and let $\mathcal{K} \subset \mathcal{T}$ be such that $\#(\mathcal{K}) = N$. Then*

$$\mathbb{E}\Big(\textit{number of colliding pairs in } \mathcal{K}\Big) \leq \frac{N(N-1)}{2M}.$$

In particular, if $M > N(N-1)/2$ then

$$P\Big(\textit{no colliding pair in } K\Big) \geq 1 - \frac{N(N-1)}{2M} > 0.$$

Proof. The expectation being a linear quantity which does not depend on independence, the first statement is again an immediate consequence of the definition of a universal family. For the second one, let us call C the number of colliding pairs. That

$$\mathbb{E}(C) = \sum_{k \geq 0} kP(C = k) = \sum_{k \geq 1} kP(C = k) \geq \sum_{k \geq 1} P(C = k) = 1 - P(C = 0),$$

from which the conclusion follows. □

In particular, if we take $M = N^2$ then $P(\text{no colliding pair in } K) \geq \frac{1}{2}$ and therefore if picking successively hash functions at random in Ω according to P we will need in expectation two tries before finding one leading to no collision [recall indeed that if a test has a probability p of success (a Bernoulli variable $\mathcal{B}(p)$) then the the number of independent tries before the first success (a Geometric variable $\mathcal{G}(p)$) has expectation $\frac{1}{p}$].

But $M = N^2$ is disappointing in terms of space needed (we would wish a table with $M = O(N)$ as anything above N can be considered a waste of space with respect to the space needed for the mere data).

We shall resolve that issue using *double hashing*. Let indeed (Ω, P) be a universal family of hash functions with the choice $M = N$. Pick a hash function h at random in Ω according to P, and denote

$$N_i := \#(h^{-1}(i)), \text{ for } i = 0, \cdots M-1 = N-1.$$

The previous lemma is of no use at the level of h, and we cannot hope the N_i to be all equal to 1 (that would correspond to a collision free hash). But for each given i, using the previous analysis we can find (and even construct) a hash function h_i (in a corresponding universal hash family (Ω_i, P_i) based on $M \equiv N_i^2$) into a table of size N_i^2 and such that

$$h_i(key_1) \neq h_i(key_2) \qquad \forall key_1 \neq key_2 \in h^{-1}(i).$$

All these tables can be viewed as sub-arrays of a large array whose total size is $\sum_i N_i^2$. The final hash function is then

1. compute $i := h(key)$
2. place key in the sub-array i at position (within the sub-array) $h_i(key)$.

By construction and by assumption on the h_i, this hash produces no collision over K. It remains to evaluation the total size $\sum_i N_i^2$. For that purpose, for $k1, k2 \in K$ let $C(k1, k2)$ denote the random variable which is equal to one if $k1$ and $k2$ collide under h and 0 otherwise. Then it is straightforward to check that, pointwise as functions over Ω,

$$\sum_{i=0}^{N-1} N_i^2 = \sum_{k1 \in K} \sum_{k2 \in K} C(k1, k2)$$

In particular, taking expectations we obtain

$$\begin{aligned}
\mathbb{E}(\sum_{i=0}^{N-1} N_i^2) &= \sum_{k1 \in K} \sum_{k2 \in K} \mathbb{E}(C(k1, k2)) \\
&= \sum_{k1 \in K} \mathbb{E}(C(k1, k1)) + \sum_{k1 \neq k2 \in K} \mathbb{E}(C(k1, k2)) \\
&\leq N + N(N-1)\frac{1}{M} = 2N - 1.
\end{aligned}$$

Recall that for a non negative random variable X and for any $c > 0$, $P(X \geq c) \leq \frac{\mathbb{E}(X)}{c}$ (this is called Markov inequality in probability, and Tchebychev inequality in measure theory). If we apply it to $\sum_{i=0}^{N-1} N_i^2$ and $c = 4N$, we obtain

$$P(\sum_{i=0}^{N-1} N_i^2 \geq 4N) \leq \frac{2N-1}{4N} \leq \frac{1}{2},$$

or conversely that

$$P(\sum_{i=0}^{N-1} N_i^2 \leq 4N) \geq \frac{1}{2}.$$

As a consequence, if we pick the initial h at random then after 2 tries in expectation we shall find one for which $\sum_{i=0}^{N-1} N_i^2 \leq 4N$, and therefore for which the corresponding final aggregated hash table will have a size less or equal to $4N = O(N)$, hence achieving our goal.

In many contexts though, the set of keys is not known prior to the choice of the hash function, and it is hopeless to avoid having to deal with collisions. We have seen how chaining can be used to deal with them. We mentioned that another solution, which often turns out more performant in practice, will be discussed later. This is our last goal for the section about hashing.

4.4 Collision work-around # 2 : open-addressing

In open addressing the hash table is exclusively based on an array, which means that colliding keys will not be inserted into linked list located in each table slot. Instead colliding keys will be dealt with by advancing in the table until a free slot is found. More precisely, to insert a new key in the table :

1. Compute `pos = hash(new_key)`
2. While `A[pos]` is occupied, increment `pos` by one and round the result modulo the table size (so that if we reach the end of the table we cycle back at the beginning of it).
3. Finally insert the key at `A[pos]` (the current value of `pos`, not the original one).

Of course this is only possible if the size of the hash table is at least as large as the number of keys it needs to store (i.e. $M \geq N$ is our previous notations), or the inserts will end-up cycling for ever without finding a free slot.

$$\text{The ratio } \frac{N}{M} \text{ is called the load factor of the table,}$$

and it must remain smaller than one. In practice it is important to keep a load factor sufficiently bounded away from 1 (e.g. 66%) or insertions will start to become costly due to the potential large number of occupied slots encountered while resolving a collision.

Care must also be taken regarding deletions. The naive solution would be to just first find the key (following the same scheme as for inserts) and then deleting it (marking the slot as empty again). This would unfortunately potentially break later look-ups. Indeed, imagine the following sequence :

1. Insert key `k1` which hashes to position `pos`.

2. Insert key `k2` which collides with `k1` and ends-up inserted at position `pos + 1`.

3. Insert key `k3` which collides with `k1, k2` and ends-up inserted at position `pos + 2`.

4. Delete key `k2`. Now the slot at position `pos + 1` is marked as free.

5. Look-up for `k3`. It hashes to `pos`, the slot is occupied, the next slot is checked and read as empty and therefore it is concluded that `k3` is not present in the table, which is obviously wrong.

To overcome this difficulty, the slots of the table will be marked either free, occupied, or deleted. The slots marked deleted are jumped over when performing look-ups, and instead they are considered as free slots when performing new insertions.

The following C code implements a dictionary (i.e. a set of distinct keys and their corresponding associated values) using an open addressing hash table. In production implementations a number of improvements are usually adopted (briefly discussed below).

data/hash_tables.c

```c
#include "hash_tables.h"

#include <stdint.h>
#include <stdlib.h>
#include <string.h>

#define FREE_SLOT 0
#define OCCUPIED_SLOT 1
#define DELETED_SLOT 2

struct HashTable *hash_table_init(size_t capacity, size_t key_len,
                                  size_t val_len)
{
        struct HashTable *ht = malloc(sizeof(struct HashTable));
        if (!ht)
                return ht;
        ht->key_len = key_len;
        ht->val_len = val_len;
        ht->size = 0;
        unsigned slot_len = 1 + key_len + val_len;
        ht->data = malloc(capacity * slot_len);
        ht->capacity = h->data ? capacity : 0;
        for (unsigned i = 0; i < ht->capacity; i++) {
                unsigned char *p = (unsigned char *)ht->data + i * slot_len;
                p[0] = FREE_SLOT;
        }
        return ht;
}

```

```
/* A general purpose hash function : FNV-1a 32 bits. Cfr :
 * https://en.wikipedia.org/wiki/Fowler%E2%80%93Noll%E2%80%93Vo_hash_function
 */
uint32_t hash_key(void *key, unsigned key_len)
{
        unsigned char *byte = key;
        uint32_t hash = 2166136261;
        while (key_len--) {
                hash ^= *byte++;
                hash *= 16777619;
        }
        return hash;
}

void *hash_table_find(const struct HashTable *ht, void *key)
{
        if (!ht || !ht->capacity)
                return NULL;
        uint32_t pos = hash_key(key, ht->key_len);
        unsigned slot_len = 1 + ht->key_len + ht->val_len;
        unsigned char *data = ht->data;
        for (size_t probe = 0; probe < ht->capacity; probe++) {
                pos = pos % ht->capacity;
                unsigned char *p = data + pos * slot_len;
                if (p[0] == FREE_SLOT) {
                        return NULL;
                }
                if ((p[0] != DELETED_SLOT) &&
                    memcmp(key, p + 1, ht->key_len) == 0) {
                        return p + 1 + ht->key_len;
                } else {
                        pos++;
                }
        }
        return NULL;
}

void hash_table_insert(struct HashTable *ht, void *key, void *val)
{
        if (ht->size >= 2 * ht->capacity / 3) {
                size_t new_cap = ht->capacity < 4 ? 8 : 2 * ht->capacity;
                hash_table_grow(ht, new_cap);
        }
        uint32_t pos = hash_key(key, ht->key_len);
        unsigned slot_len = 1 + ht->key_len + ht->val_len;
        unsigned char *data = ht->data;
        for (size_t probe = 0; probe < ht->capacity; probe++) {
                pos = pos % ht->capacity;
                unsigned char *p = data + pos * slot_len;
                if (p[0] == FREE_SLOT) {
                        memcpy(p + 1, key, ht->key_len);
                        memcpy(p + 1 + ht->key_len, val, ht->val_len);
```

```
82                          ht->size++;
83                          p[0] = OCCUPIED_SLOT;
84                          return;
85                  } else {
86                          pos++;
87                  }
88          }
89          /* Hash table is full */
90          printf("Hash table is full ! Implement hash_table_grow "
91                 "or initialize with a larger capacity.\n");
92          abort();
93  }
94
95  static void hash_table_grow(struct HashTable *ht, size_t new_cap)
96  {
97          // Homework ! Note: requires rehashing all keys.
98          // 1. Save the address ht->data for later use.
99          // 2. Init a new table with new_cap capacity (that will
100         //    overwrite ht->data)
101         // 3. Traverse the old table, read its data and insert it
102         //    (e.g. through hash_table_insert) into the new table.
103         // 4. When done, free the old data
104 }
105
106 void hash_table_delete(const struct HashTable *ht, void *key)
107 {
108         // Homework !
109 }
110
111 void hash_table_fini(struct HashTable *ht)
112 {
113         ht->size = 0;
114         ht->capacity = 0;
115         free(ht->data);
116 }
117
118 #undef FREE_SLOT
119 #undef OCCUPIED_SLOT
120 #undef DELETED_SLOT
```

data/hash_tables.c

As already mentioned the previous implementation, although avoiding linked lists, can be improved in a number of ways.

1. If the table size is required to be a power of two, then it is possible to replace the modulo operation by a bitwise operation (which even on today's architecture is substantially less costly). Indeed, due to integer representation if M is a power of two then modulo M amounts to bitwise AND with $M - 1$ (think about it if it isn't immediately clear, $M - 1$ in such a case is a sequence of zero bits followed by a sequence of one bits, as many as the correspond power of two M is).

2. The linear probing (that is the fact that if slot `pos` is occupied we advance to `pos + 1`) can be replaced by a quadratic probing. The latter corresponds to advancing to `pos + probe`, where `probe` is the probe number. In other words, the first position checked if `pos` is occupied is `pos + 1` (first probe). If is is also occupied we jump to `pos + 1 + 2` (second probe), etc to `pos + 1 + 2 +... + k` until (say) we find a free slot at probe number k. Quadratic probing has the advantage that it avoids clustering of occupied cells after collisions (it spreads new probes further away wrt linear probing). It must only be used when the first optimization above applies, i.e. with tables whose length is a power of two. The reason is that when M is a power of two the mapping `probe` $\rightarrow$ `pos + probe(probe+1)/2 modulo M` induces a bijection from $\{0, \cdots, M-1\}$ into itself (this is not immediate, we did the proof in class but it isn't particularly enlightening, so I skip it here). For M not a power of 2, it is generally not the case, and the table may then appear full to the algorithm (because not all cells would be visited by the jump process) although it isn't.

3. The occupancy status byte of each slot can be avoided by reserving (whenever possible) two keys in the set of all potential keys to represent free and deleted slots. This not only saves one byte (which often isn't a big deal since keys and values generally occupy more than that) but often offers some alignment optimizations to the compiler, especially with the next optimization.

4. Generic programming in C is convenient and acceptably fast, but type erasure (i.e. use of `void*` and `memcpy, memcmp`) prevent the compiler from potential optimizations possible when the type of the data is known at compile type. C++, through the use of templates, can be used to overcome this.

The next C++code snippet shows all these optimizations working together in a hash look-up function. The types of the keys (and values not shown here) are templates to be filled by the user at the time of the hash-table instantiation (we shall discuss that in two weeks). The hashing is delegated to a hasher type (another template parameter) which must implement, in addition to `hash`, the `is_equal` and `is_empty` functions. Note the look-up function does not return a value here, but simply the index in the table (the user can read at that slot index to decide what to do (insert/delete/whatever)).

```
1  template<typename K, typename H>
2  static inline size_t hash_lookup(K *keys, size_t buckets, H hasher, K key)
3  {
4          /* In debug mode, assert the table size is indeed a power of two */
5          assert(((buckets - 1) & buckets) == 0);
6
7          size_t mask = buckets - 1;
8          size_t bucket = hasher.hash(key) & mask;
9
10         for (size_t probe = 0; probe < buckets; probe++) {
```

```
11
12                  if (hasher.is_empty(keys[bucket]) ||
13                                  hasher.is_equal(keys[bucket], key)) {
14                          return bucket;
15                  }
16                  /* quadratic probing */
17                  bucket = (bucket + probe + 1) & mask;
18          }
19
20          /* Should never reach this point */
21          assert(false && "Table is full !\n");
22          return 0;
23  }
```

5 Trees

5.1 Some definitions and generalities

Let V be a finite set, and $E \subseteq V \times V$. The elements in V are called vertices (or nodes) and those in E are called edges. Whenever $e = (v_1, v_2) \in E$, we say that v_1 is a parent of v_2, and that v_2 is a child of v_1.

Definition. (V, E) is a rooted tree with root $r \in V$ if and only if

1. all nodes in $V \setminus \{r\}$ have exactly one parent.
2. the root r has no parent.

By convention, an empty set of nodes and edges is also called a rooted tree (with no root). Nodes in the tree that have non children are called leaves.

A number of easy properties or new definitions are in order :

- For every $v \in V$, there exists a unique $n \in \mathbb{N}$ and a unique path

$$r = e_0 \to e_1 \to \cdots \to e_n = v$$

  such that for each $0 < i < n-1$, $(e_i, e_{i+1}) \in E$. The length n of the path is called the depth of the node v.

- By definition[8] the height of a rooted tree is zero if it is empty or else one plus the largest depth among its nodes (or equivalently among its leaves) if not. It is therefore also the number of visited nodes in the longest path in the tree.

- Given $v, w \in V$, v is called an ancestor of v if w belongs to the unique path joining the root to w. Inversely, w is then called an descendent of v.

- For $v \in V$, the *sub-tree rooted at* v is the tree which has for vertex set $V' = \{v' \in V \text{ s.t. } v' \text{ is a descendent of } v\}$ and for edge set $E' = \{(v', w') \in E \text{ s.t. } v' \in V',\ w' \in V'\}$.

Definition. A binary tree is a rooted tree for which each node as at most two children.

Since there are at most two children per node in binary trees, it is common to think of their nodes as having two slots: one for the so-called left children and the other for the so-called right children. These slots can be occupied or empty. Accordingly, each node $v \in V$ possesses a (possibly empty) left sub-tree, noted $lst(v)$, and a (possibly empty) right sub-tree, noted $rst(v)$. These sub-trees are respectively rooted at the left and right children of v, when the latter exist.

[8] Some authors prefer a different convention which differs by one, the empty tree having a height of -1

Searching into trees will imply traversing them down from the root. In applications, it is therefore desirable to keep their height under control. If a tree contains $N = \#(V)$ nodes, then its height H can be as large as $N - 1$ (when the tree is no more than an linked list). On the extreme opposite, if a binary tree is perfect (i.e. if all its leaf nodes are at the same depth and all non leaf nodes have exactly two children), then $N = 1 + 2^1 + 2^2 + \cdots + 2^{H-1} = 2^H - 1$. In particular $H = \log_2(N + 1)$ for such trees. Perfect trees are often too constrained to be useful. The following balanced trees will both be flexible enough and have a sufficiently good upper bound on their height.

Definition. A binary tree is called balanced if for each $v \in V$, the height of its left and right sub-trees differ at most by one.

Lemma 4. *If a binary tree is balanced, then its height H and its total number of nodes N satisfy that*

$$N \geq F_{H+1} + 1,$$

where $(F_k)_{k\geq 0}$ is the Fibonacci sequence : $F_0 = 0$, $F_1 = 1$, and $F_k = F_{k-1} + F_{k-2}$ for $k \geq 2$.
In particular

$$H = O(\log N)$$

as $N \to +\infty$.

Proof. Let's call $T(h)$ the minimal number of nodes in a balanced binary tree of height $h \geq 0$. Clearly $T(0) = 0$, $T(1) = 1$, and for $h \geq 2$

$$T(h) \geq 1 + T(h-1) + T(h-2).$$

Indeed, the left and right sub-trees of the root must have heights equal to either $(h - 1, h - 1)$, or $(h - 1, h - 2)$ or $(h - 2, h - 1)$. Since T is clearly increasing, the claimed inequality follows. If we note $S(h) = T(h) + 1$ then we obtain

$$S(h) \geq S(h-1) + S(h-2) \qquad \forall h \geq 2,$$

with $S(0) = 1$ and $S(1) = 2$. It follows that $S(h) \geq F_{h+1}$, and hence the first claim in the statement. The Fibonacci sequence can be written in matrix form

$$\begin{pmatrix} F_{k+1} \\ F_k \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} F_k \\ F_{k-1} \end{pmatrix},$$

and therefore also

$$\begin{pmatrix} F_{k+1} \\ F_k \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}^k \begin{pmatrix} F_1 \\ F_0 \end{pmatrix}.$$

The eigenvalues of the matrix in the above expression are given by $\lambda_\pm = \frac{1\pm\sqrt{5}}{2}$ and therefore as $k \to +\infty$

$$\frac{F_k}{\lambda_+^k} \to c > 0$$

(eigenvectors must be computed to obtain c explicitly), which implies that

$$log(F_k) = k \log(\lambda_+) + o(1) \text{ as } k \to +\infty,$$

and the second claim follows as well. □

In the sequel we shall restrict our attention to two families of binary trees that have important applications as data structures : binary search trees (BST) and binary heaps.

5.2 Binary search trees (BST)

Binary search trees are important alternatives to hash-tables for storing keys or key/-value pairs. While keys were hashed into hash tables, keys shall be sorted into binary search trees. More precisely :

Definition. A binary search tree is a binary tree for which each node is associated with a key and the following BST condition holds :

1. $\forall v \in V$, $\forall w \in lst(v)$, $w.key < v.key$
2. $\forall v \in V$, $\forall w \in rst(v)$, $w.key > v.key$.

In particular, keys must be distinct[9].

Finding a key in a BST is therefore as simple as :

- Start at the root.
- Go down the three by choosing the left of right sub-tree at each encountered node by comparing the looked-up key with the key of the node.
- When a leaf node is reached then new node is inserted as its left or and the key has still not been found then it isn't in the tree.

Insertions are very similar :

- Start at the root.
- Go down the three by choosing the left of right sub-tree at each encountered node by comparing the key to be inserted with the key of the node.
- Insert the key as a new node (which shall be a leaf) when the are no more sub-tree to visit reaching an .

[9]Although, there are ways to circumvent this limitation in practice, it is a good exercise to think about it

The following simple implementation is based on recursion. The values here are assumed to be integers for simplicity. They might be replaced by any type together with an ordering. In the tutorials, you will deal with a situation where the tree nodes are contained in the data (this is called an intrusive tree), rather containing it, it is a much more common use in real applications, which also has the advantage to delegate memory allocation to the user side. Note also that in this implementation we allow nodes with equal values.

```c
#include <stdlib.h>
#include <stdbool.h>

struct Node {
        int val;
        struct Node *child[2]; /* 0 = left, 1 = right */
};

static struct Node *new_node(int val)
{
        struct Node *n = malloc(sizeof(struct Node));
        n->val = val;
        n->child[0] = n->child[1] = NULL;
        return n;
}

struct Node *bst_find_recur(struct Node *root, int val)
{
        if (!root)
                return root;
        return bst_find_recur(root->child[val > root->val], val);
}

/* Note : In this implement duplicate vals are allowed */
struct Node *bst_insert_recur(struct Node *root, int val)
{
        if (!root) {
                root = new_node(val);
        } else {
                bool dir = val > root->val;
                root->child[dir] = bst_insert_recur(root->child[dir], val);
        }
        return root;
}
```

The case of deletions are slightly less obvious. In some implementations the node is so-called “lazy deleted”, which means it is marked as deleted but not actually removed, and its key value is kept for later routing. Otherwise, the proper way to do it is to swap the node to be deleted with either the smallest node in its right sub-tree, or the

largest node in its left sub-tree (and delete the latter). There is a possible short-cut in the case where the node to be deleted only has one (or zero) children : in that case it suffices to deleted the node and attach its (only or none) children to its grand parent.

```
struct Node *bst_delete_recur(struct Node *root, int val)
{
        if (!root)
                return root;
        if (root->val != val) {
                bool dir = val > root->val;
                root->child[dir] = bst_delete_recur(root->child[dir], val);
        } else if (!root->child[0] || !root->child[1]) {
                bool dir = !root->child[0];
                struct Node *tmp = root->child[dir];
                free(root); /* might be null */
                root = tmp;
        } else {
                /* Smallest node in the root right sub-tree */
                struct Node *tmp = root->child[1];
                while (tmp->child[0]) {
                        tmp = tmp->child[0];
                }
                /* Steal it */
                root->val = tmp->val;
                root->child[1] = bst_delete_recur(root->child[1], tmp->val);
        }
        return root;
}
```

The following variants avoid the use of recursion, this can be more efficient when the tree becomes deeper. The lack of recursion implies that equivalent of parent pointers must be kept and updated during the traverse down.

```
struct Node *bst_find(struct Node *root, int val)
{
        struct Node *n = root;
        while (n && n->val != val) {
                n = n->child[val > n->val];
        }
        return n;
}

struct Node *bst_insert(struct Node *root, int val)
{
        struct Node *nn = new_node(val);
        if (!root) {
                return nn;
```

```
15          }
16
17          struct Node *n = root;
18          int dir = val > n->val;
19
20          while (n->child[dir]) {
21                  n = n->child[dir];
22                  dir = val > n->val;
23          }
24
25          n->child[dir] = nn;
26          return root;
27  }
28
29  struct Node *bst_delete(struct Node *root, int val)
30  {
31          struct Node *del = root;  /* node to delete */
32          struct Node *pdel = NULL; /* parent of node to delete */
33          int dir;
34          while (del && del->val != val) {
35                  dir = val > del->val;
36                  pdel = del;
37                  del = del->child[dir];
38          }
39          if (!del)
40                  return root;
41
42          struct Node *rep; /* replacement node */
43          if (!del->child[0]) {
44                  rep = del->child[1];
45          } else if (!del->child[1]) {
46                  rep = del->child[0];
47          } else {
48                  rep = del->child[1];
49                  struct Node *prep = del; /* parent of replacement node */
50                  while (rep->child[0]) {
51                          prep = rep;
52                          rep = rep->child[0];
53                  }
54                  if (prep != del)
55                          prep->child[0] = rep->child[1];
56          }
57          if (del != root) {
58                  pdel->child[dir] = rep;
59          } else {
60                  root = rep;
61          }
62          free(del);
63          return root;
64  }
```

Average time complexity. It is clear from the implementations that the costs of lookups/insert/delete are directly proportional to the height of the tree. If the tree ends-up being very unbalanced (e.g. if the keys are inserted in order or in reverse order, leading to a height $H = N - 1$), there will be no advantage of a tree over a list. The following theoretical result shows that in the mean (i.e. averaging over all possible shuffling of the input keys), insertion costs are logarithmic.

First, without loss of generality we can assume that set of keys to be inserted are the integers $\{1, \cdots, N\}$. Indeed, the actual keys do not matter, only their ordering is important. Our averaging set will therefore be the set $\sigma_N = \{\sigma : \{1, \cdots, N\} \to \{1, \cdots, N\} \text{ a permutation}\}$, equipped with uniform probability.

Lemma 5. *The expectation of the total insertion cost of all the keys starting from an empty BST is $O(N \log N)$.*

As a consequence, the average cost per inserted key is $O(\log N)$.

By total insertion cost, we mean here the total number of comparisons (i.e. of routing) necessary for the whole process.

Proof. The key observation in order to count the number of comparisons during insertions is the following claim :

Claim 1. Let $1 \leq i < j \leq N$. The keys i and j are compared at most once during the whole process, and they are compared if and only if there does not exist $i < k < j$ such that $\sigma(k) < \sigma(i)$ and $\sigma(k) < \sigma(j)$.

Indeed, first notice that i and j can only be compared during the insertion of the one of the two that is inserted last (i.e. the one which has the largest value under σ). Next, the keys are be compared if and only if they were not already sent into two different sub-trees by an earlier inserted key. By the BST property, such a dividing key can only be of the form k with $i < k < j$, which proves the claim.

Claim 2. Let $1 \leq i < j \leq N$. Then the probability (according to σ_N equipped with the uniform probability) that there exist no $i < k < j$ such that $\sigma(k) < \sigma(i)$ and $\sigma(k) < \sigma(j)$ is equal to $2/(j - i + 1)$.

Indeed, by symmetry, among the $j - i + 1$ numbers $i, \cdots, j$, all have the same probability (thus equal to $1/(j-i+1)$) to be the one which as the smallest value under σ . Therefore the probability that the one with the smallest value of σ within $i, \cdots, j$ is either i or j is exactly $2/(j - i + 1)$, which proves the second claim.

Now the expectation of the total insertion cost is, by linearity of expectation :

$$\sum_{i<j} \frac{2}{j - i + 1}.$$

We can compute the previous sum explicitly :

$$\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\frac{2}{j-i+1}=\sum_{i=1}^{N-1}\sum_{k=2}^{N-i+1}\frac{2}{k}=\sum_{k=2}^{N}\sum_{i=1}^{N-k+1}\frac{2}{k}=\sum_{k=2}^{N}\frac{2(N-k+1)}{k}$$
$$=2(N+1)\sum_{k=2}^{N}\frac{1}{k}-2(N-1)=2(N+1)\sum_{k=1}^{N}\frac{1}{k}-4N.$$

In the above, we have used the change of unknown $k=(j-i+1)$ in the first equality and the Fubini theorem for series for the second equality, the remaining ones being straightforward. Since the harmonic series $\sum_{k=1}^{N}\frac{1}{k}=\log(N)+O(1)$ as $N\to+\infty$, the conclusion follows. □

It can also be proved, but it is less immediate, that under the same setting the expectation of the height of the BST after insertion is also of order $\log(N)$. This information is of similar nature but is not equivalent to the total insertion cost.

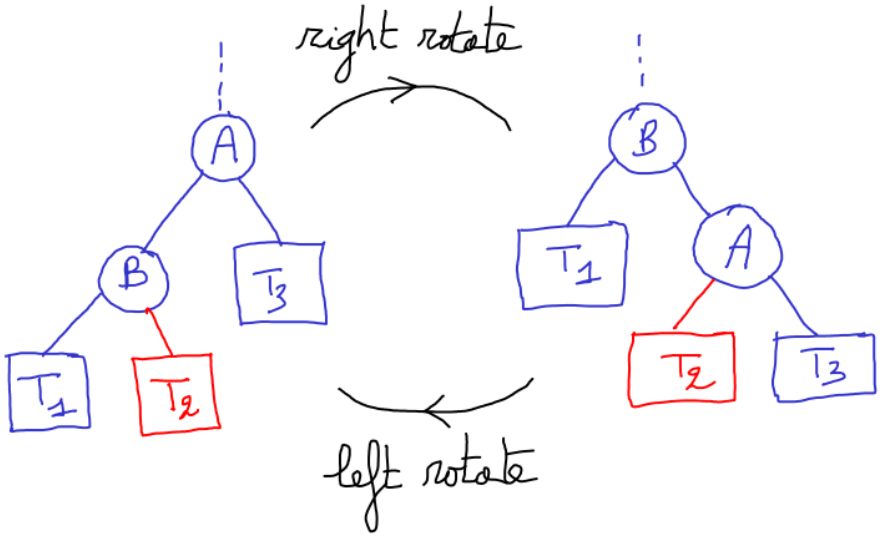
5.3 Self balancing BST

Although the average time complexity for insertions has been shown to be $O(\log(N)$ in average, if we are unlucky the total cost could be as bad as N. For that reason, our goal in this section is to present a modification of the insertion and deletion processes that will have the following features :

- They are compatible with the BST property.
- They have (together with lookups) a guaranteed time complexity of $O(\log N)$ where N is the number of nodes in the tree at the time of the insertion/deletion/lookup.

The key modification is a number of so-called rotations of the tree after an insertion or a deletion in order to maintain a balanced tree. If this property can be maintained, then we already know that the tree height will be $O(\log(N))$ and therefore so will be the cost of insertions/deletions/lookups.

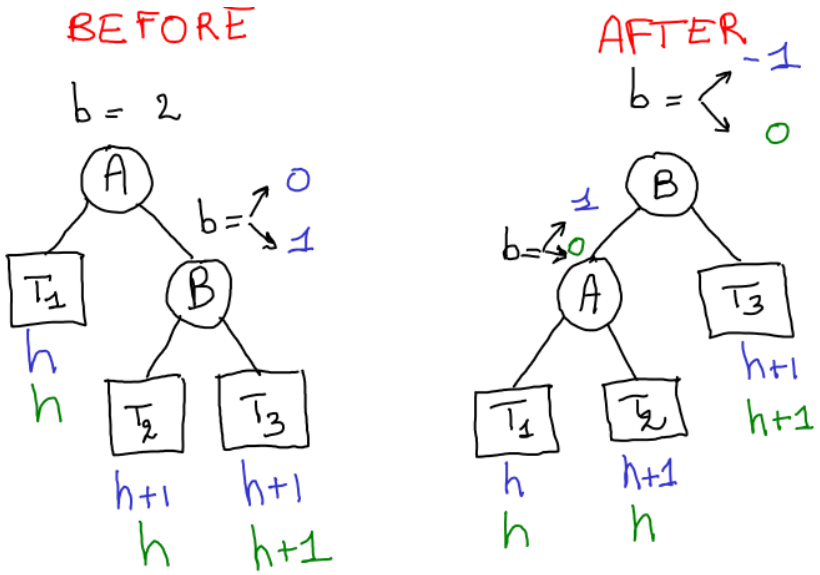
Rotations are described in the following figure :



In this figure, the round shapes represent tree nodes, while the square shapes represent their (potentially empty) left of right sub-trees. During rotation, the node A and B exchange their parent/child relation. Since the one that becomes the new parent can only keep at most two children (to remain a binary tree), it must detach one of its sub-trees and reattach it to the one that becomes a child. There is only one of such sub-trees that can be exchanged (T_2 in the figure) in order to maintain the BST property : all the nodes in T_2 are larger (in the sense of their key value) than B and smaller than A, both before and after the rotation.

It remains to explain how to maintain a balanced tree using rotations after an insertion or a deletion. The first observation is that if the tree was balanced before the insertion/deletion, the balance factors of the nodes in the tree after the operation can only belong to the set $\{-2, -1, 0, 1, 2\}$. Indeed, sub-trees heights are modified at most by one unit when inserting or deleting a node. Among these cases, only the ones with balance factors ± 2 require some rebalancing. In the sequel we assume therefore that some node in the tree, let's call it A, has a balance factor ± 2. We also assume that A has the biggest depth among the unbalanced nodes (the other ones shall be treated after). By symmetry, we can also assume that the balance factor of A is $+2$, the case -2 being perfectly left/right symmetrical. Since the balance of A is positive, the node A must necessarily have a right child, let's call it B. We shall distinguish two cases depending on the balance factor of B (by assumption B is balanced since it has higher depth than A).

Case 1 : The balance factor of B is non negative.
In tat case we perform a single right rotation as in the figure below :

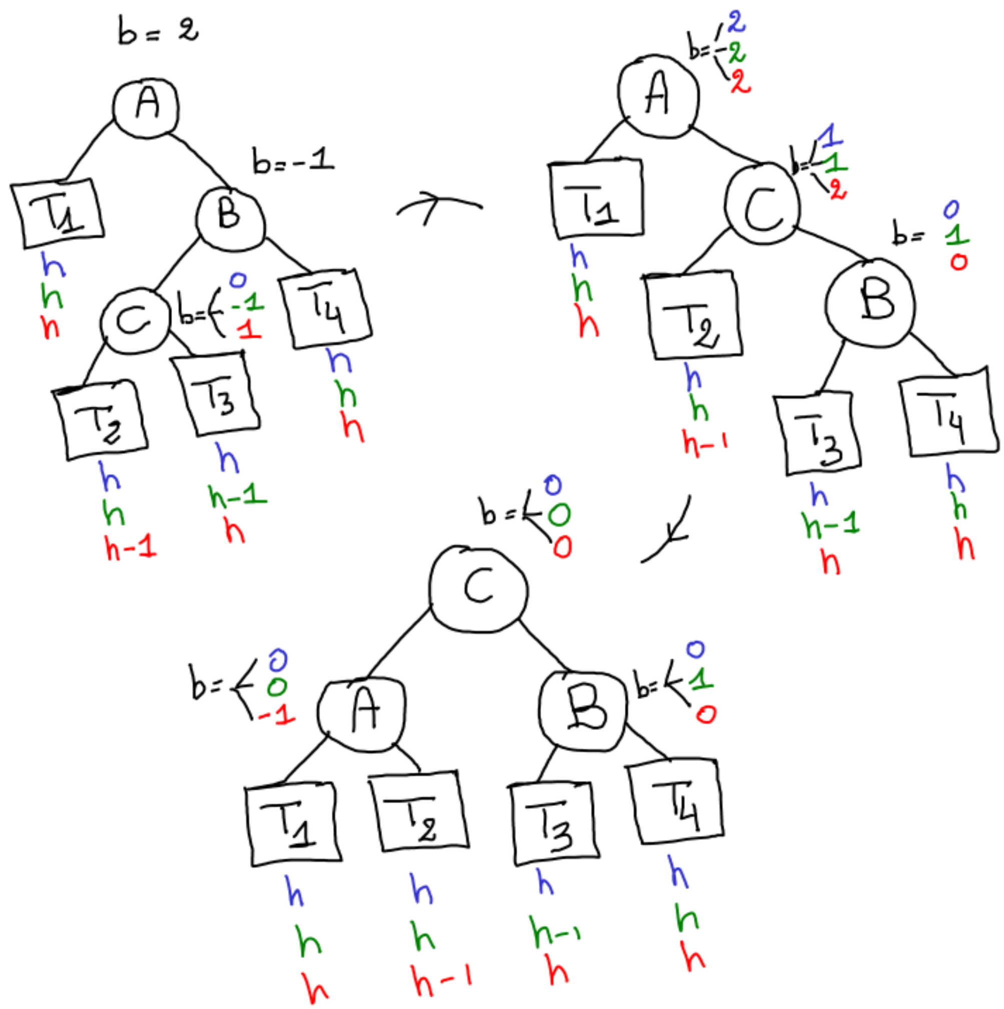


We have noted h the height of the left sub-tree of A (T_1), the other sub-tree heights have been deduced depending on the balance factor of B. We observe that after rotation, both A and B are balanced.

Note also that only the green case can occur after an insertion leading to an unbalance. Indeed, in the blue case the sub-trees T_2 and T_3 both have a height $h+1$, and therefore at least one of them had a height of $h+1$ before the insertion and then unbalance would have already been present. The consequence of this is that the height of the tree rooted at B after rotation is exactly the same (i.e. $h+2$) as the height of the tree rooted at A before rotation and before the insertion took place (i.e. when T_3 had height h and not $h+1$). This implies that the balance factor of the nodes higher up in the tree are unaffected by the insert, and therefore that **at most one node can be unbalanced after an insertion leading to Case 1**. The same applies for deletions, except that both the blue and green cases can occur. In the blue case both the tree after rotation and the tree before deletion (i.e. for which T_1 had height $h+1$) have total height $h+3$, while in the green case they both have height $h+2$. Therefore **at most one node can become unbalanced after a deletion leading to Case 1.**.

Case 2 : The balance factor of B is negative (and hence -1).

In that case we perform a double rotation as in the figure below. Note that since B is left heavy, it must have a left child which we call C.



Here also we noted h the height of the left sub-tree of A, and deduced the other possible heights based on the balance factors. In the three colored cases, the height of the tree rooted at C after the double rotation is always $h+2$. Similar reasoning as above leads to the following : only the green and the red cases can occur for insertions, and they correspond to situations where prior to insertion the height of the tree rooted at A was $h+2$. Hence the total height of the tree does not change after insertion + rebalancing, and therefore **at most one node can be unbalanced after an insertion leading to Case 2**. The three colored cases can occur for deletions (i.e. when T_1 had height $h+1$ prior to deletion), but here the height of the tree before deletion was different and equal to $h+3$, so we cannot unfortunately conclude that rebalancing will occur only at one node for deletions. However, the only nodes that can necessitate rebalancing are the ones along the path from the root to the deleted nodes, and these are at most $O(\log(N))$ since the tree is balanced.

The trees which are maintained balanced following the above procedure are called AVL trees (abbreviation for their inventors G. Adelson-Velsky and E. Landis). Sum-

marizing we have :

Proposition 1. *The cost for insertions/deletions/lookups in an AVL tree is always* $O(\log(N))$*, where* N *is the number of nodes present in the tree. After an insertion, at most one node may necessitate rebalancing.*

We finish this section with an extension of our previous implementation of BST to the case of AVL.

```
1  #include <assert.h>
2  #include <stdlib.h>
3
4  struct AVLNode {
5          int val;
6          struct AVLNode *child[2]; /* 0 = left, 1 = right */
7          int height; /* Height of the tree rooted at this node */
8  };
9
10 static struct AVLNode *new_node(int val)
11 {
12         struct AVLNode *n = malloc(sizeof(struct AVLNode));
13         n->val = val;
14         n->height = 1;
15         n->child[0] = n->child[1] = NULL;
16         return n;
17 }
18
19 static int get_balance(struct AVLNode *root)
20 {
21         if (!root)
22                 return 0;
23         int left = root->child[0] ? root->child[0]->height : 0;
24         int right = root->child[1] ? root->child[1]->height : 0;
25         return right - left;
26 }
27
28 static void update_height(struct AVLNode *root)
29 {
30         if (!root)
31                 return;
32         int left = root->child[0] ? root->child[0]->height : 0;
33         int right = root->child[1] ? root->child[1]->height : 0;
34         root->height = 1 + (left > right ? left : right);
35 }
36
37 /* dir : 0 (false) = left, 1 (true) = right */
38 static struct AVLNode *rotate(struct AVLNode *root, bool dir)
39 {
40         assert(root);
41         struct AVLNode *next_root = root->child[!dir];
```

```
42          assert(next_root);
43          struct AVLNode *tmp = next_root->child[dir];
44          root->child[!dir] = tmp;
45          next_root->child[dir] = root;
46          update_height(root);
47          update_height(next_root);
48          return next_root;
49  }
50
51  struct AVLNode *fix_balance(struct AVLNode *root)
52  {
53          int b = get_balance(root);
54          if (abs(b) <= 1)
55                  return root;
56          /* dir = heavy direction = ! rotate direction */
57          bool dir = b > 0;
58          int b2 = get_balance(root->child[dir]);
59          bool dir2 = b2 > 0;
60          if (b2 && (dir != dir2))
61                  root->child[dir] = rotate(root->child[dir], !dir2);
62          root = rotate(root, !dir);
63  }
64
65  struct AVLNode *avl_find(struct AVLNode *root, int val)
66  {
67          if (!root)
68                  return NULL;
69          return avl_find(root->child[val > root->val], val);
70  }
71
72  struct AVLNode *avl_insert(struct AVLNode *root, int val)
73  {
74          if (!root) {
75                  root = new_node(val);
76          } else {
77                  bool dir = val > root->val;
78                  root->child[dir] = avl_insert(root->child[dir], val);
79                  update_height(root);
80                  root = fix_balance(root);
81          }
82          return root;
83  }
84
85  struct AVLNode *avl_delete(struct AVLNode *root, int val)
86  {
87          if (!root)
88                  return NULL;
89          if (root->val != val) {
90                  bool dir = val > root->val;
91                  root->child[dir] = avl_delete(root->child[dir], val);
92          } else if (!root->child[0] || !root->child[1]) {
93                  bool dir = !root->child[0];
```

```
94                  struct AVLNode *tmp = root->child[dir];
95                  free(root); /* might be null */
96                  root = tmp;
97          } else {
98                  /* Smallest node in the root right subtree */
99                  struct AVLNode *tmp = root->child[1];
100                 while (tmp->child[0]) {
101                         tmp = tmp->child[0];
102                 }
103                 /* Steal it */
104                 root->val = tmp->val;
105                 root->child[1] = avl_delete(root->child[1], tmp->val);
106         }
107         if (!root)
108                 return NULL;
109         update_height(root);
110         root = fix_balance(root);
111         return root;
112 }
```

5.4 Binary heaps (and Heap sort)

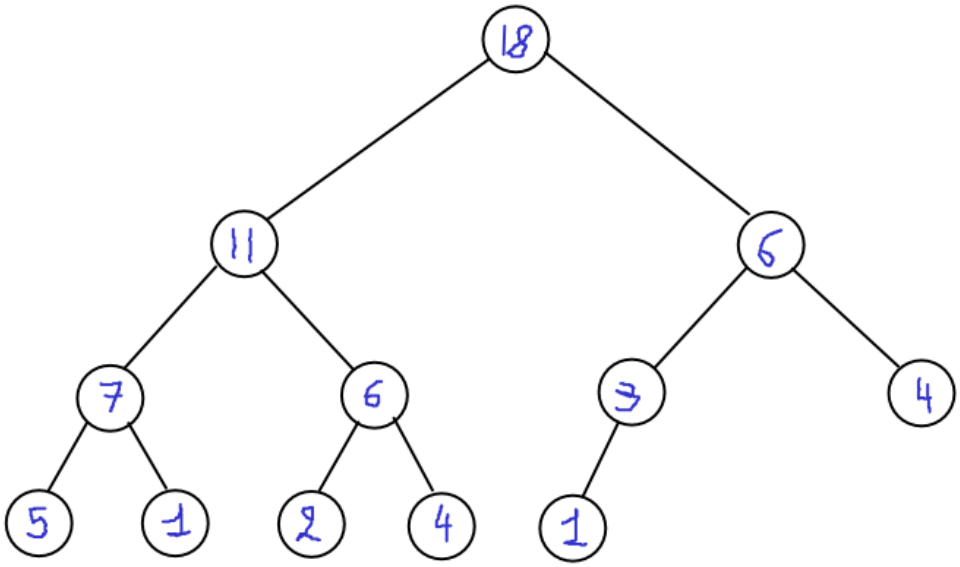
Definition. A (max on top) binary heap is a rooted binary tree where each node is associated with key and the following heap property holds :

1. $\forall v \in V$, $\forall w \in lst(v)$, $w.key <= v.key$.
2. $\forall v \in V$, $\forall w \in rst(v)$, $w.key <= v.key$.

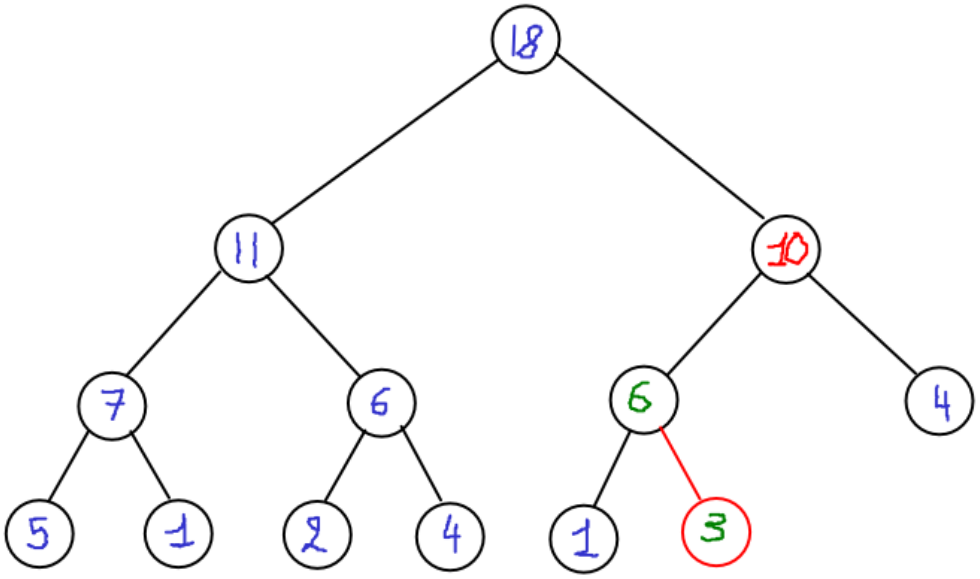
By reversing all inequalities in the definition we would obtain a (min on top) binary heap. The theory for both being completely parallel, it is common to restrict to one of them.

In a sense, the heap replaces the left to right ordering of BST by a top to bottom ordering. This change is more profound than it looks at first, in particular one cannot easily perform a lookup of a key in a heap, because there is no routing rule which can tell us whether to search in the left or right child (we just know the keys in both subtrees are smaller or equal to the key at the visited node). For insertion, on contrary the freedom is greater, since the heap property only tells us if we need to proceed down, but if yes we can proceed left or right as we please. As a matter of fact, heap type data structures generally only implement lookup or extraction of the highest key, that is the one at the root, and insertion of an arbitrary key (also, contrary to BST, keys in heaps may not be unique). Heaps are typically used for implementing priority-queues, where extraction of the task with highest priority is the only deletion op available, while tasks of arbitrary priorities can be inserted.

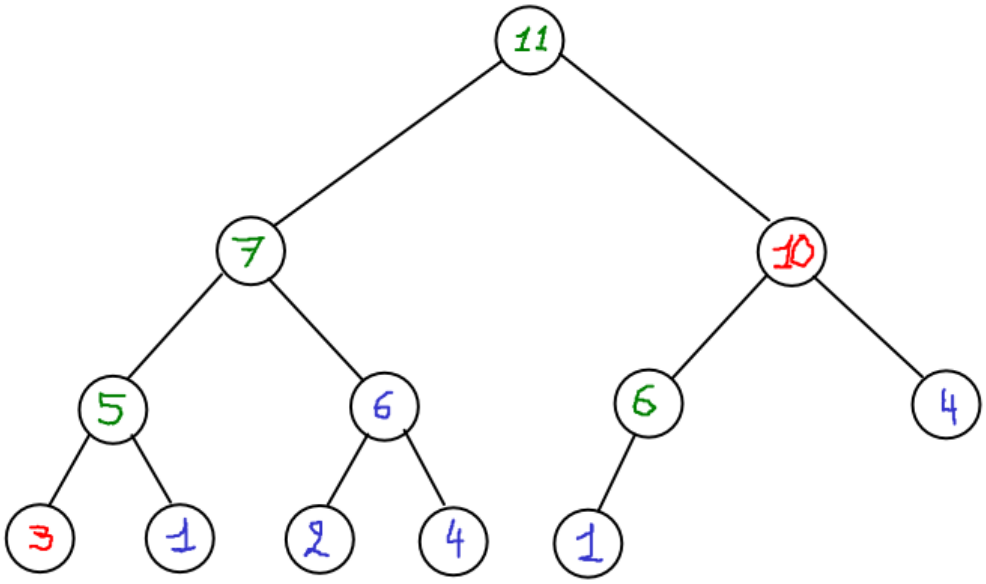
Because there is more freedom during insertion in heaps, the resulting tree can be chosen to not only be balanced but also complete and full on the left. This means that all depth levels in the binary tree are full except possibly the one, corresponding to the highest depth, and which must only be full from the left. An example is illustrated in the next figure :



Under this restriction, the position of of a newly inserted node is completely constrained and must occur at the "lower-right" position in the tree. Since this may break the heap property, the newly inserted node is swapped with its parent in the tree as long as the heap property is not satisfied : this is called a *sift-up* of the node. The next figure illustrate the result of this process after a new node of value 10 as been inserted in the heap.



When extracting the root node, the constraint to be a complete tree forces the "lower-right" node in the tree to moved in place of the old root. This again breaks the heap property and the new root must be pushed down a number of time in order to reset it. The correct governing rule for the push down is to swap the node with the one of its two children which has the highest value (choosing the one with the lowest value may imply another failure of the heap property), as long as the heap property isn't satisfied. This is again illustrated in the last figure below, we the heap is shown after the root 18 was extracted :



The most interesting feature concerning this restriction about the tree to be a complete tree is that that such trees can easily be implemented as arrays, thus avoiding the

use of pointers and allocation at each insertion. In this array implementation, the root node is placed at index 0, and the next indices in the array correspond to reading the tree from top to bottom and on each depth level from left to right. Under this rule, the child-parent relation translates into the following simple expressions where i refer to indices in the array :

- `parent(i) = (i - 1) / 2`
- `left_child(i) = 2 * i + 1`
- `right_child(i) = 2 * i + 2`

The cost if insertion or extraction of the root in a heap, as in the case of balanced tree, is $O(\log(N))$. This cost correspond to the maximum number of swaps which occur during each of such operations, and is bounded by the total height of the tree, which is $O(\log(N))$.

The C code for such implementations is the object of one of the tutorials, with an additional feature to allow for node value update, which will be helpful when implementing the Dijkstra algorithm for finding optimal paths in weighted graphs.

6 Graphs

Definition. A graph $G = (V, E)$ is given by a set V, whose elements are called the vertices (or the nodes) or the graphs, and a subset $E \subseteq V \times V$, whose elements are called the edges of the graph.

In the sequel, we shall always implicitly assume, whenever we consider a graph $G = (V, E)$, that the set V (and hence E) is a finite set. The notations $|V|$ and $|E|$ will be used to refer to the cardinality of V and E respectively, and when this is convenient we shall label the vertices in V from 1 to $|V|$.

Since $E \subseteq V \times V$ it always holds that $0 \leq |E| \leq |V|^2$. A graph is called sparse if $|E|$ is "much smaller" than $|V|^2$, and many important cases we have $|E| = O(|V|)$ (in particular when the *degree* of each vertex, that is the number of incoming edges into that vertex, is bounded a priori).

Also since $E \subseteq V \times V$, the listing order of an edge end-points matters, and for that reason graphs with the abode definition are often called *directed* graphs. A graph is called *undirected* if for all $(v, v') \in E$, the reverse edge (v', v) also belongs to E.

6.1 Graph representation

Often in implementation, once the vertex set V is given, the edge set is not described as an abstract set of edges but using one or the other of the following two structures :

i) The adjacency matrix This is the square $|V| \times |V|$ matrix A for which

$$A_{ij} = 1 \text{ if } (i, j) \in E \text{ else } 0.$$

With this representation, the graph is undirected if and only if the adjacency matrix is symmetric. The advantage of this representation is that it allows for easy modification of the connectivity (i.e. adding or removing edges), since it only amounts to changing some values between 0 and 1. The disadvantage of that representation is that it requires $O(|V|^2)$ memory. For sparse graphs, it therefore represents a substantial waste of space (the matrix is sparse, in the sense that it mostly contain zeros), and this is the reason why the second representation below is favoured in such cases. As a matter of fact, in scientific computing a number of important spare graphs come from sparse matrices (e.g. the matrices used in solving partial differential equations using finite differences or finite elements), and such matrices, are encoded using some a variation of the representation below.

ii) The adjacency lists In that case, for each vertex i ($1 \leq i \leq |V|$) the list

$$Adj(i) := \{i \in 1, \cdots, |V| \text{ s.t. } (i, j) \in E\}.$$

is formed. That representation is therefore only a partition of E according to a key which is the starting vertex of each edge. The spatial complexity is $O(|V| + |E|)$ (the total length of the lists is $|E|$ but even empty lists must be noticed as such, the reason

for the $|V|$ term). Note that although we refer to adjacency *lists*, if the graph is not going to be modified these lists can be packed into a small number of arrays as e.g. in the following C struct :

```
1 struct Graph {
2         int nv;
3         int ne;
4         int *counts;
5         int *offsets;
6         int *edges;
7 };
```

In the above, $nv = |V|$, $ne = |E|$, `counts` is an array of size nv where $\texttt{counts}[i]$ contains the number of outgoing edges at vertex i (here $0 \leq i < nv$). The array `offsets` is also of size nv and

$$\texttt{offsets}[i] = \sum_{j=0}^{i-1} \texttt{counts}[j].$$

Finally, the array `edges` is of size ne and for $0 \leq i < nv$,

$$Adj(i) = \{edges[k], \text{ s.t. } \texttt{offsets}[i] \leq k < \texttt{offsets}[i] + \texttt{counts}[i]\}.$$

Although the above representation is quite general, there are cases where an a priori knowledge about the graph allows for variants with slightly better performance or information content. We have seen an example in the tutorials when when built what we called an adjacency table for a conformal triangular mesh. In that situation, we knew that each triangle (viewed here as a node of a graph) has at most three neighbors (an edge of that graph corresponds to a common edge (in the mesh sense here!) shared by the two triangles, with opposite edge orientations). This is the reason why we encoded all the adjacency information in a single array of size $3 * ntri$, with the additional information that a triangle is on the boundary of the mesh if and only if one of its potential three neighbors is absent (marked with a -1 in the implementation we made).

6.2 Graph traversal # 1 : Breadth First Search (BFS)

We shall consider two important families of graph traversal, the so-called *Breadth first search*, and *Depth first search*. Starting from a source vertex, the first one will grow a front by visiting first all vertices that are sufficiently close (in the sense of the minimal number of edges necessary to join them from the source) to the source. The second one, in contrast, tries to advance as deep as possible in the graph starting from the source,

and then comes back and visit different branches when it reaches leaves or already visited nodes.

The idea of breadth first search is elementary : visit neighbors of the sources, and then neighbors of the neighbors, etc. Care must be taken in order to avoid visiting vertices many times, and also about the possibility to reach all vertices in that way (graph connectivity).

Algorithm 5 Breadth first search from source vertex s

```
function BFS(s)
    create and empty queue Q
    enqueue s and mark s as visited
    while Q not empty do
        dequeue front element v from Q
        for all w ∈ Adj(v) do
            if w is not marked visited then enqueue w and mark it as visited
            end if
        end for
    end while
end function
```

The previous will only visit some vertex v if there exists a path in G from s to v. If one wishes to visit all the vertices of the graph then the following encapsulating function can be used :

Algorithm 6 Breadth first search full traversal

```
function BFS
    Mark all vertices v as non visited
    for all v ∈ V do
        if v is not marked visited then BFS(v)
        end if
    end for
end function
```

The first important remark that one should make about BFS is that by construction each vertex v is enqueued at most once (and exactly once in the second version) in Q. In particular the while loop, and therefore also the algorithm terminates, and after at most $|V|$ runs of the loop. The time complexity of this traversal is thus easily computed as $O(|V| + |E|)$.

6.3 Application to shortest path

We show next a first easy application of BFS to the shortest path problem.

Definition. A path in G is a sequence of vertices $(v_i)_{0\leq i\leq \ell}$ in V such that

$$v_i \neq v_{i+1} \text{ and } (v_i, v_{i+1}) \in E \ \forall\, 0 \leq i < \ell.$$

The number ℓ is called the length of that path, and the path is said to join v_0 to v_ℓ.

Given a source vertex $v \in V$, we define the subset

$$Reach(v) = \{w \in V \text{ s.t. there exists a path in } G \text{ joining } v \text{ to } w\}.$$

If the graph G is undirected, then the relation $w \in Reach(v)$ defines and equivalence relation, and the equivalence classes are called the connected components of the graph G. For directed graphs, the above relation is in general not symmetric, and connected components have no universal definition. Yet it always holds that

$$\forall\, u, v, w \in V,\ \Big(v \in Reach(u) \text{ and } w \in Reach(v)\Big) \Rightarrow w \in Reach(u).$$

Definition. For $v \in V$ and $w \in Reach(v)$, we set

$$\delta(v, w) = \inf\{\ell \in \mathbb{N}, \text{ s.t. there exists a path } (v_i)_{0\leq i\leq \ell} \text{ in } G \text{ joining v to w}\}.$$

When the graph G is undirected, the function δ defines a distance on the connected components of G. In the general directed graph case, δ is also in general not symmetric, but still is satisfies the following triangle type inequality :

Lemma 6. *Let $u \in V$, $v \in Reach(u)$, and $w \in Reach(v)$, then*

$$\delta(u, w) \leq \delta(u, v) + \delta(v, w).$$

The proof by contradiction is elementary, and shows moreover that whenever $(v_i)_{0\leq i\leq \ell}$ is some shortest path in G joining v_0 to v_ℓ, then for all $0 \leq j \leq k \leq \ell$ the subsequence $(v_i)_{j\leq i\leq k}$ is also a shortest path in G joining v_j to v_k.

The following slight extension of the $BFS(s)$ breadth first search traversal will solve the problem of finding shortest paths starting at a source vertex s :

- add a `.dist` integer attribute to each vertex (can be implemented using an array of size $|V|$ of distances instead of attributes). For visited vertices, this attribute will eventually contain the minimal distance from the source s to that vertex.
- add a `.pred` attribute to each vertex (can also be implemented with an array instead of additional attributes). For visited vertices, this attribute will eventually refer to the predecessor of that vertex in the shortest path to v found by the algorithm.
- the source s is initially set with $s.dist = 0$.
- whenever we enqueue some vertex $w \in Adj(v)$, we set $w.dist = v.dist + 1$ and $w.pred = v$.

Proposition 2. *A target vertex $t \in V$ gets discovered by $BFS(s)$ if and only if $t \in Reach(s)$. Moreover, for such vertices the value $t.dist$ contains the actual minimal distance from s to t in G, i.e.*

$$t.dist = \delta(s,t).$$

Besides, one (among) shortest path(s) from s to t is obtained (in reverse order) by recursively taking the .pred attribute of the vertices starting from t and until s is reached.

Proof. i)It is immediate by construction that discovered vertices are all in $Reach(s)$. The reverse inclusion can easily be proved by induction on the value of $\delta(s,t)$. If $\delta(s,t) = 0$ then $t = s$ and thus t is discovered by $BFS(s)$ (at initialization). Assume next that for some $k \in \mathbb{N}$ all vertices in $Reach(s)$ having $\delta(s,v) \leq k$ are discovered by $BFS(s)$, and let $t \in Reach(s)$ such that $\delta(s,t) = k+1$. Let $(v_i)_{0 \leq i \leq k+1}$ be a shortest path in G joining $v_0 = s$ to $v_{k+1} = t$. By induction we know that v_k, which satisfies $\delta(s,v_k) = k$ by a property mentioned above (a sub path of a shortest path is a shortest path), gets discovered by $BFS(s)$. But then since $v_{k+1} \in Adj(v_k)$, at the time v_k is dequeued, the vertex v_{k+1} is (enqueued and) marked discovered. This proves the first set equality.

ii) We next show that $t.dist \geq \delta(s,t)$, for all $t \in Reach(s)$. This is easily proved by induction on the value of $t.dist$. If $t.dist = 0$ and $t = s$ and therefore $t.dist = 0 = \delta(s,s) = \delta(s,t)$. Assume next that for some $k \geq 0$ we have $t.dist \geq \delta(s,t)$ for all $t \in Reach(s)$ such that $t.dist \leq k$. Let $t \in Reach(s)$ be such that $t.dist = k+1$, and let $u := t.pred$. By construction, we have $u.dist = k$ and therefore by induction we know that $u.dist \geq \delta(t,u)$. Since $t \in Adj(u)$ we have $t \in Reach(u)$ and by Lemma 6

$$t.dist = u.dist + 1 \geq \delta(s,u) + 1 = \delta(s,u) + \delta(u,t) \geq \delta(s,t).$$

iii) We finally show that $t.dist = \delta(s,t)$, for all $t \in Reach(s)$. Assume by contradiction that this is false, and let $t \in Reach(s)$ be a vertex for which equality fails, and among these one with the smallest value (noted ℓ) of $\delta(s,t)$. By construction and ii), we necessarily have

$$\ell = \delta(s,t) \leq t.dist - 1.$$

Let $(v_i)_{0 \leq i \leq \ell}$ be a shortest path in G joining s to t, and let $v := v_{\ell-1}$. By the sub path optimality property we have $\delta(s,v) = \ell - 1$ and therefore by the minimality assumption about t we have $\delta(s,v) = v.dist$. At the time v is discovered by BFS(s), we distinguish two cases. Case 1: t is not yet discovered. In that case following BFS(s) we should have set $t.dist = v.dist + 1$. But then $t.dist = v.dist + 1 = \delta(s,v) + 1 = \ell = \delta(s,t)$, which contradicts the (by contradiction) assumption. Case 2: t was already discovered. That instead would lead to the conclusion that $t.dist \leq v.dist$ (see hereafter), and therefore $t.dist \leq v.dist = \delta(s,v) = \delta(s,t) - 1$, which again is a contradiction. The fact that $t.dist \leq v.dist$ when t is discovered before v is a consequence of the fact that each step in BFS(s) the values of the *.dist* attribute are naturally ordered within the queue Q, with the smallest values on the front (i.e. dequeue) side and the larger values on the

tail (i.e. enqueue) side, and with at most a difference of 1 between the largest and the smallest values. This is easily proved by induction on the number of dequeues already done during BFS(s), and the fact that when we dequeue a vertex, the non discovered vertices are enqueued with a .dist value increased by one. □

6.4 Weighted shortest path : the Dijkstra algorithm

In this section we shall add a weight function over edges $W : E \to \mathbb{R}_+^*$, and we define accordingly a weighted shortest path distance for $s \in V$ and $t \in Reach(s)$:

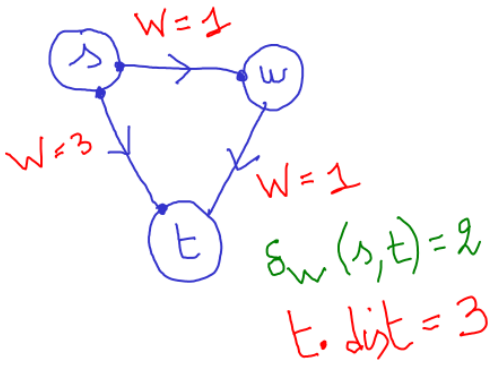
$$\delta_W(s,t) = \inf \Big\{ \sum_{i=0}^{\ell-1} W(v_i, v_{i+1}) \Big\},$$

where the infimum is taken over paths in G joining s to t. The unweighted case of the previous section hence corresponds to the case $W \equiv 1$.

It is tempting, in view of the discussion in the previous section, to simply replace in the BFS(s) enqueue operations the setting $w.dist = v.dist + 1$ by

$$w.dist = v.dist + W(v,w).$$

The following simple example shows that this wouldn't yield the equality $t.dist = \delta_W(s,t)$ is all cases.



If we examine the proof of Proposition 2, the only place where the adaptation from δ to δ_W would fail is at the very last step when we argued that the values of $.dist$ are naturally ordered in the queue from front to tail, and that as a consequence the values of $.dist$ are increasing as a function of their time of dequeue. To remedy to this failure, the simplest and most effective way, as suggested by Dijkstra in 1959, is to replace the queue Q by a heap H, with the minimal value of $.dist$ on top. More precisely, the Dijkstra algorithm starting at vertex s is :

Algorithm 7 Dijkstra from source vertex s

```
function DIJKSTRA(s)
    create and empty queue H
    push s into H with .dist = 0 and mark s as discovered
    while H not empty do
        pop minimal element v from H
        mark v as visited
        for all w ∈ Adj(v) do
            if w is not marked discovered then
                push w into H with w.pred = v and w.dist = v.dist + W(v, w)
            else if w.dist > v.dist + W(v, w) then
                update w.dist = v.dist + W(v, w) and w.pred = v in H
            end if
        end for
    end while
end function
```

We have

Proposition 3. *A target vertex $t \in V$ gets discovered by Dijkstra(s) if and only if $t \in Reach(s)$. Moreover, for such vertices the value $t.dist$ contains the actual minimal weighted distance from s to t in G, i.e.*

$$t.dist = \delta_W(s,t).$$

Besides, one (among) shortest path(s) from s to t is obtained (in reverse order) by recursively taking the .pred attribute of the vertices starting from t and until s is reached.

Proof. As already mentioned the proof is an almost immediate adaptation of the one of Proposition 2, we repeat it for completeness, except for part i) which is really identical and can still be performed by induction on $\delta(s,t)$ (instead of $\delta_W(s,t)$ which wouldn't fit an induction stricto sensu).

ii) We next show that $t.dist \geq \delta_W(s,t)$, for all $t \in Reach(s)$. We argue by contradiction and consider that smallest value of $t.dist$ for which $t.dist < \delta_W(s,t)$. The vertex t cannot be equal to s because $s.dist = \delta_W(s,s) = 0$. Therefore t possesses a valid $u := t.pred$ and by construction $t.dist = u.dist + W(u,t)$. Since W is positive (this is one of the few places where it matters), we have $u.dist < t.dist$ and therefore by minimality $u.dist = \delta_W(s,u)$. This in turn implies that $\delta_W(s,t) > t.dist = u.dist + W(u,t) = \delta_W(s,u) + W(u,t) \geq \delta_W(s,u) + \delta_W(u,t)$, which contradicts the triangle inequality for δ_W.

iii) We finally show that $t.dist = \delta(s,t)$, for all $t \in Reach(s)$. Assume again by contradiction that this is false, and let $t \in Reach(s)$ be a vertex for which equality fails,

and among these one with the smallest value (noted d) of $\delta_W(s,t)$. By construction and ii), we necessarily have

$$d = \delta_W(s,t) < t.dist.$$

Let $(v_i)_{0\leq i\leq \ell}$ be a shortest path in G joining s to t, and let $v := v_{\ell-1}$. By the sub path optimality property we have $\delta_W(s,v) = d - W(v_{\ell-1} < d$ and therefore by the minimality assumption about d we have $\delta_W(s,v) = v.dist$. At the time v is marked *visited* by BFS(s), we distinguish two cases.
Case 1: t is not yet visited. In that case following BFS(s) we should have set $t.dist = v.dist + W(v,t)$ (if t was also not discovered) or $t.dist = \min(t.dist, v.dist + W(v,t))$ (in case t was already discovered). Besides, the value of $t.dist$ could then only have been lowered later in an update, and the value of $v.dist$ will no longer change since by assumption v was just visited. Therefore eventually we would still have $t.dist \leq v.dist + W(v,t)$. But then $t.dist \leq v.dist + W(v,t) = (d - W(v,t)) + W(v,t) = d = \delta_W(s,t)$, which contradicts the (by contradiction) assumption.
Case 2: t was already visited. That instead would lead to the conclusion that $t.dist \leq v.dist$ (see hereafter), and therefore $t.dist \leq v.dist = \delta_W(s,v) = \delta_W(s,t) - W(v,t) \leq \delta_W(s,t)$, which again is a contradiction. The fact that $t.dist \leq v.dist$ when t is marked visited before v is a consequence of the fact that at each step in BFS(s) the smallest $.dist$ value in the heap is extracted (by definition of min heap extraction), and the values that are (potentially) then pushed or updated in the heap are strictly larger than the extracted one, because W was assumed positive. □

We finish by discussing the time complexity of the Dijkstra algorithm. For that purpose, we assume that the heap H is implemented as a binary complete tree, as we have seen in the corresponding section. Since H contains, at any time during the algorithm, at most $|V|$ elements, the cost of each operation (push, pop, or update) is at most $O(\log(|V|))$. Also, there are at most $|V|$ push and pop operations, and at most $|E|$ update operations. The total time complexity is therefore $O((|V| + |E|)\log(|V|))$.

6.5 Graph traversal # 2 : Depth First Search (DFS) (TODO)

6.6 Application to Topological sort (TODO)

6.7 Graph cuts and minimal spanning trees (TODO)

7 Meshes (TODO)

7.1 Conforming meshes

7.2 Adjacency tables

7.3 Boundary and geometric invariants

8 Sparse matrices (TODO)

8.1 Representations

8.2 Computations

8.3 Band width reduction

9 Spatial data structures (TODO)

9.1 Spatial hashing

9.2 K-d trees

9.3 R-trees