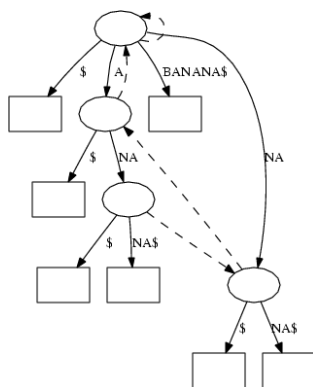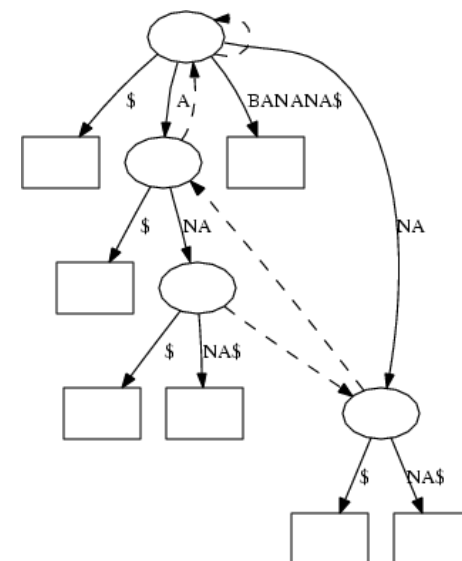# Further Mathematics and Algorithms

Lesson 1: *Use Data Structures and Algorithms!*

Course structure, examples of data structures and algorithms

Outline

1. **Course structure**

2. Example of Using DSA

3. Sophisticated Program

4. State-of-the-Art

Welcome to Further Mathematics and Algorithms

- First 7 weeks Daniela and I will be teaching you about algorithms

- The last 4 weeks you will learn some further maths

- I'm teaching you algorithms (and data structures) in C++

- My ambition is not only to teach you data structures and algorithms academically but also to get to a new level of coding in C++

Quick Survey on C++

- Who considers themselves a competent coder in C++?

- Who knows what a class constructor is?

- Who knows what a default constructor is?

- Who is happy using templates?

- Who understands pointers?

- Who knows what the key word `explicit` means?

- Who has heard of *resource acquisition is initialisation (RAII)?*

Recommended Course Text
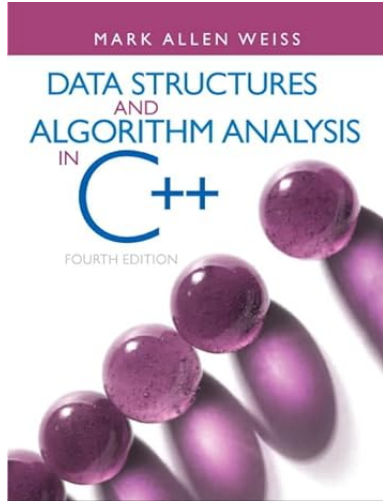
- *Data Structures and Algorithm Analysis in C++* by M. A. Weiss

  - ⋆ Best introduction to Data Structures and Algorithms
  - ⋆ Not huge, but covers all the basics

- Available in the library

What is a Data Structure?

any of various methods of organising data items (as records) in a computer

- Container for data

- E.g. sets, stacks, lists, trees, graphs

- Clean interface, e.g. `push`, `pop`, `delete`

- Usually designed for fast or convenient access

What is an Algorithm?

a sequence of unambiguous instructions for solving a problem, i.e. for obtaining a required output for a legitimate input in a finite amount of time

- E.g. `sort, search, match`

- Well defined and generic

- Guarantees on performance

Exemplary OO-Software

- Abstraction from details of problem

- Declaration of intention

- Clean interfaces

- Hidden implementations

- Makes programs readable and maintainable

- Reuse code—don't even have to write it yourself

  Thou shall not re-implement common data structures

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Example: Sort program
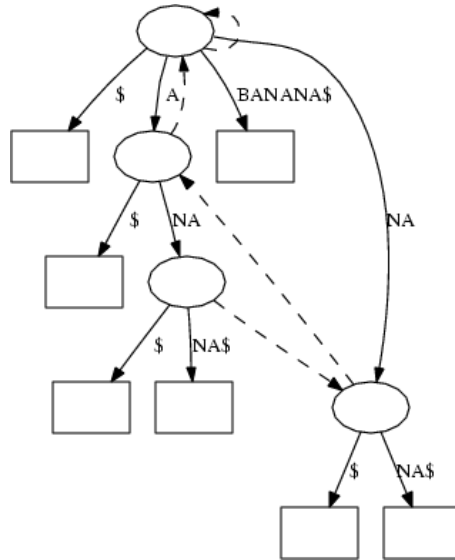
- Suppose we want to write a program to

  ⋆ read an input file of integers
  ⋆ sort the integers
  ⋆ write a list of integers to standard out

- In Unix there is a command called `sort` which does just this

- Note that you don't know the number of inputs

Code for sort

```cpp
#include <iostream>
#include <fstream>

int main(int argc, char** argv) {
  std::ifstream myfile(argv[1]);

  int array_size = 10;
  int* array = new int[array_size];
  int cnt = 0;
  while(myfile.good()) {
    if (cnt==array_size) {
      int* new_array = new int[2*array_size];
      for(int i=0; i<array_size; ++i)
        new_array[i] = array[i];
      delete[] array;
      array = new_array;
      array_size *= 2;
    }
    myfile >> array[cnt++];
  }
```

```cpp
  for(int i=0; i<cnt; ++i) {
    int index = 0;
    for(int j=1; j<cnt-i; ++j) {
      if (array[j]<array[index])
        index = j;
    }
    std::cout << array[index] << std::endl;
    array[index] = array[cnt-i-1];
  }
}
```

Notes on Code

- Details of code don't matter

- Simple program (~ 20 lines of code)

- Uses a simple array

- Difficult to see what is going on

- On 10 000 inputs it takes 10 seconds to run

Using Data Structures and algorithms

```cpp
#include <iostream>
#include <fstream>
#include <iterator>
#include <vector>
#include <algorithm>
using namespace std;

int main(int argc, char *argv[])
{
  ifstream in(argv[1]);
  vector<int> data;
  copy(istream_iterator<int>(in), istream_iterator<int>(),
       back_inserter(data));
  sort(data.begin(), data.end());
  copy(data.begin(), data.end(), ostream_iterator<int>(cout,"\n"));
}
```

Sorting Doubles

```cpp
#include <iostream>
#include <fstream>
#include <iterator>
#include <vector>
#include <algorithm>
using namespace std;

int main(int argc, char *argv[])
{
  ifstream in(argv[1]);
  vector<double> data;
  copy(istream_iterator<double>(in), istream_iterator<double>(),
       back_inserter(data));
  sort(data.begin(), data.end());
  copy(data.begin(), data.end(), ostream_iterator<double>(cout,"\n"));
}
```

Notes on C++

- `vector<int>` is the C++ standard resizable array

- input/output is treated as a copy

- Code is easy to read

  - ⋆ Declare `vector<int>` or `vector<double>`
  - ⋆ copy input file into vector
  - ⋆ sort vector
  - ⋆ copy sorted vector to standard output stream

- On 100 000 inputs takes 10ms to run

# Summary: Why use Data Structures?

Data structure version is

- Easier/quicker to code■

- More readable (less bugs)■

- Easier to modify and change■

- Easier to port to another language■

- Better (in this case faster)■

Outline

Sophisticated Programs

- Data structures and algorithms allow moderately competent programmers to write some very impressive programs■

- E.g. consider a program to count all occurrences of words in a document■

- We want to output the words in sorted order■
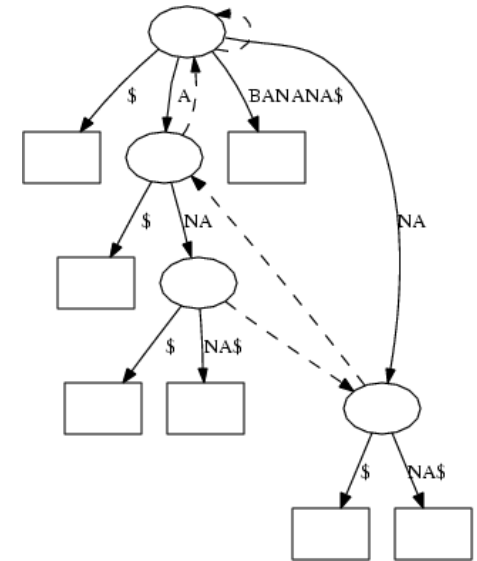
countWords

```cpp
#include <stuff>

int main(int argc, char** argv) {
  ifstream in(argv[1]);
  map<string, int> words;

  string s;
  while(in >> s) {
    ++words[s];
  }

  vector<pair<string,int> > pairs;
  copy(words.begin(), words.end(), back_inserter(pairs));
  sort(pairs.begin(), pairs.end(),
    [](auto& a, auto&b){return a.second>b.second;});

  for(auto w=pairs.begin(); w!=pairs.end(); ++w) {
    cout << w->first << "_occurs_" << w->second << "_times\n";
  }
}
```

Using countWords

```
> countWords text.dat | more
the occurs 97 times
of occurs 96 times
to occurs 57 times
and occurs 42 times
a occurs 36 times
be occurs 31 times
will occurs 26 times
we occurs 23 times
that occurs 23 times
is occurs 21 times
have occurs 19 times
freedom occurs 18 times
```

Programming Challenge

- Run on "I have a dream" speech with 1550 words in 0.02 seconds

- Challenge for good programmers

  Write a program without use data structures in less that 10 times as much code that runs in less than 10 times as long

- Probably possible, but certainly not easy—almost certainly take you 10 times longer to code

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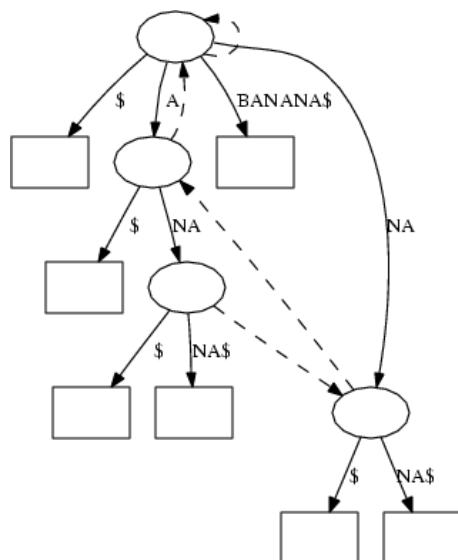
DNA Sequencing

- In modern whole shotgun genome sequencing the full genome is broken into small pieces

- The pieces are then read by a sequencing machine

- This reads short sections (around 1000) bases

- The reads are then assembled to construct the full genome

Sequencing and Assembly

ATACCACCATGCCTCCTTGCTCCAATATTAATTCAAGGCG
ATACCACCATGCCTCCTTGCTCCAATATTAATTCAAGGCG
ATACCACCATGCCTCCTTGCTCCAATATTAATTCAAGGCG
ATACCACCATGCCTCCTTGCTCCAATATTAATTCAAGGCG
ATACCACCATGCCTCCTTGCTCCAATATTAATTCAAGGCG

ATACCACCATGCCTCCTTGCTCCAATATTAATTCAAGGCG

TTGCT	TACCA	CAAGG	TTAAT	TTCAA	TCCTT
TGCCT	AATAT	CCTCC	AGGCG	ATACC	ACCAT
CTCCT	CCTTG	ATGCC	GCTCC	TGCCT	TTGCT
TGCTC	ACCAC	TTGCT	AATAT	CAAGG	TGCCT
TACCA	CACCA	CCTTG	CTCCA	TATTA	AATTC

New Generation Sequencers

- The estimated cost of sequencing the human genome in 2005 was $10 000 000

- To reduce the cost there was and is a drive to produce new sequencing machines

- These tend to read much shorter sections of DNA (e.g. 20-100nt)

- Can these be assembled?

Repeats
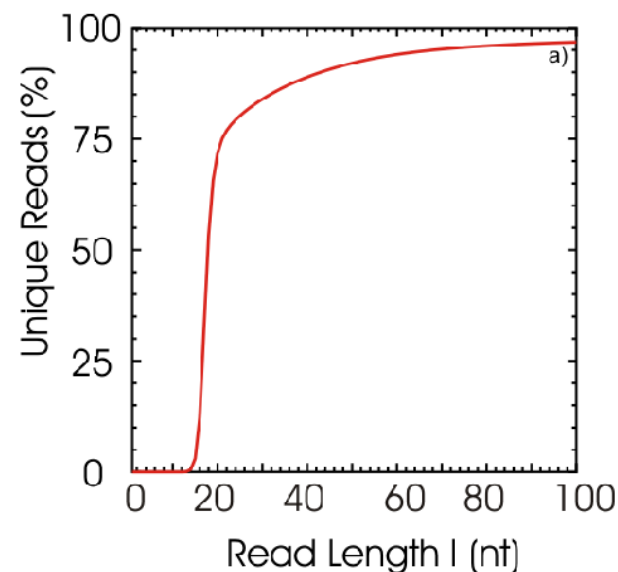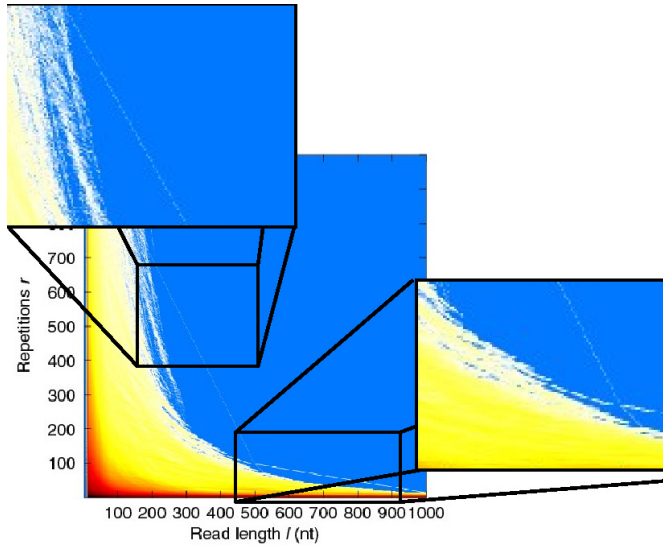
- The difficulty of assembly is caused by repeats

  ATACCACCATGCCTCCTTGCTCCAATCCACCATCAAGGCG

- How many repeats are there in the human genome? (Incidentally the human genome is 3.2 billion base **pairs**)

- This is an important question for developing new sequencing technologies

Repeats in Human Genome

Repeats Structure

Computing Repeats

- A naive program would take n^2 operations where $n = 6.4 \times 10^9$

- If we used this we would still be waiting for the program to finish

- Could not answer this question a few years ago—not because computers weren't powerful, but because the algorithms had not been developed

- Used state-of-the-art suffix arrays

- Smart algorithms allow you to do things which you cannot do otherwise

To Use DSA You Need To

- Know what common data structures and algorithm do

- Understand the implementations enough to modify existing data structures to be fit for purpose

- Understand time/space complexity to select the right data structure or algorithm

- Understand software interfaces for DSA

- Be able to combine data structures

- The rest of this course teaches you these skills