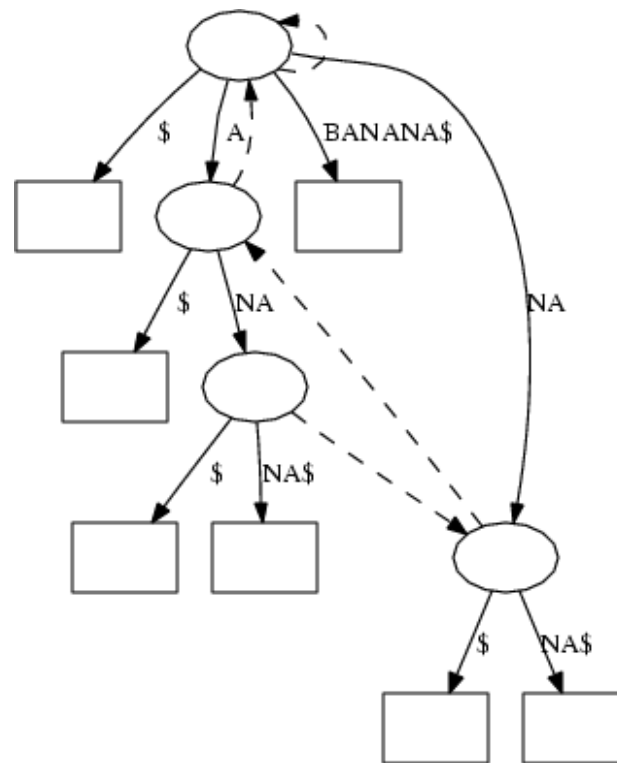


# Further Mathematics and Algorithms

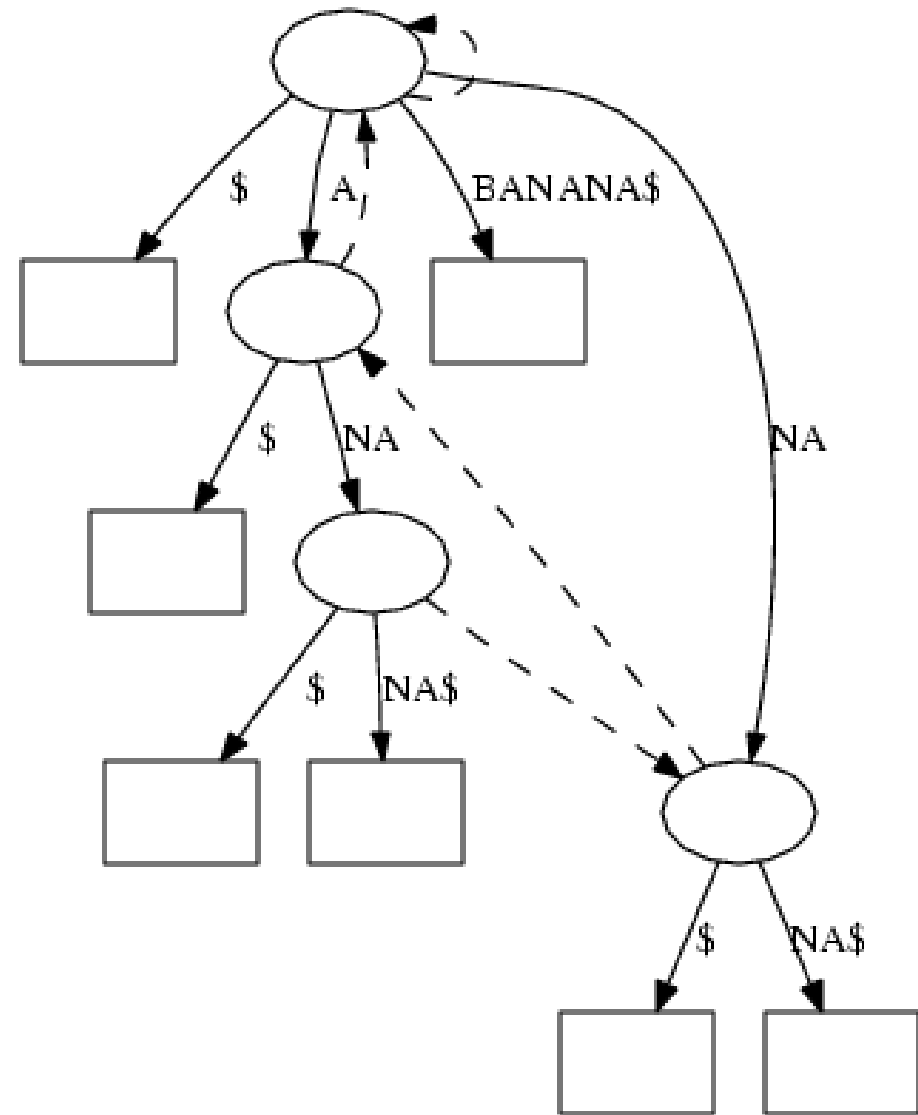
## Lesson 1: *Use Data Structures and Algorithms!*



*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

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# Quick Survey on C++

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



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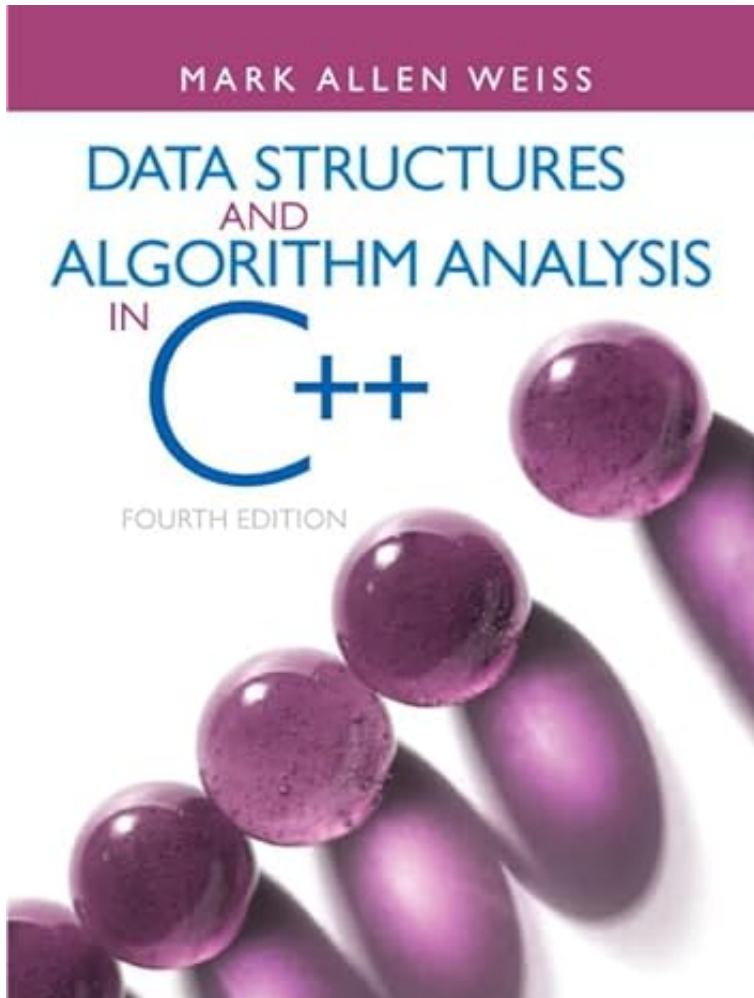
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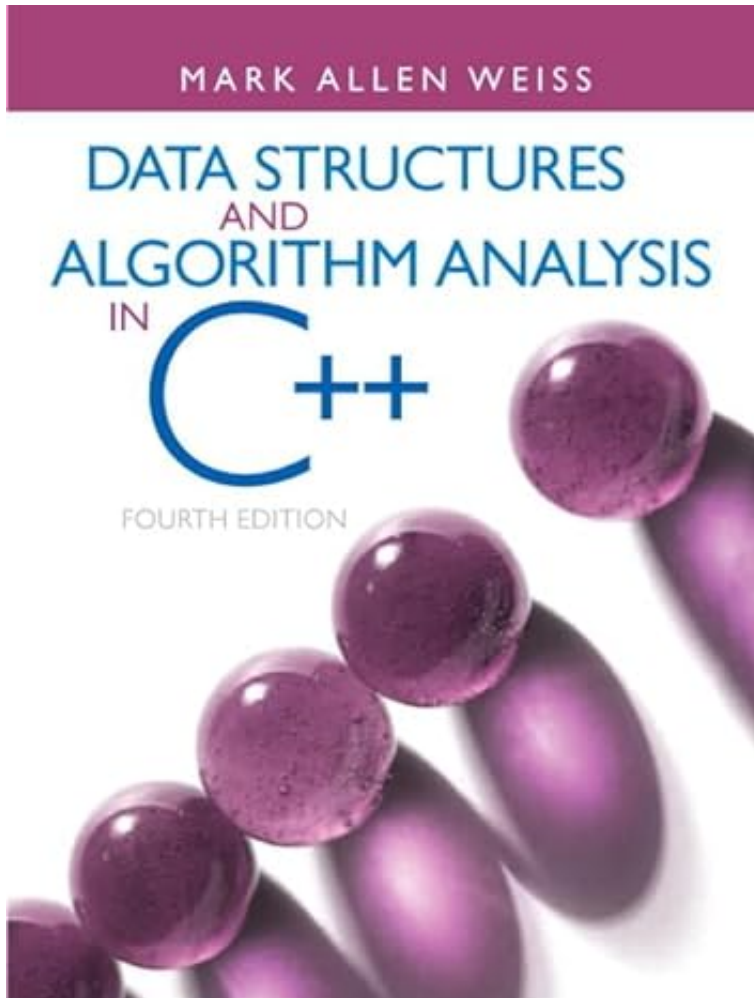
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- Who knows what the key word `explicit` means?
- Who has heard of *resource acquisition is initialisation (RAII)*?

# Recommended Course Text



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  - ★ Best introduction to Data Structures and Algorithms
  - ★ Not huge, but covers all the basics
- Available in the library

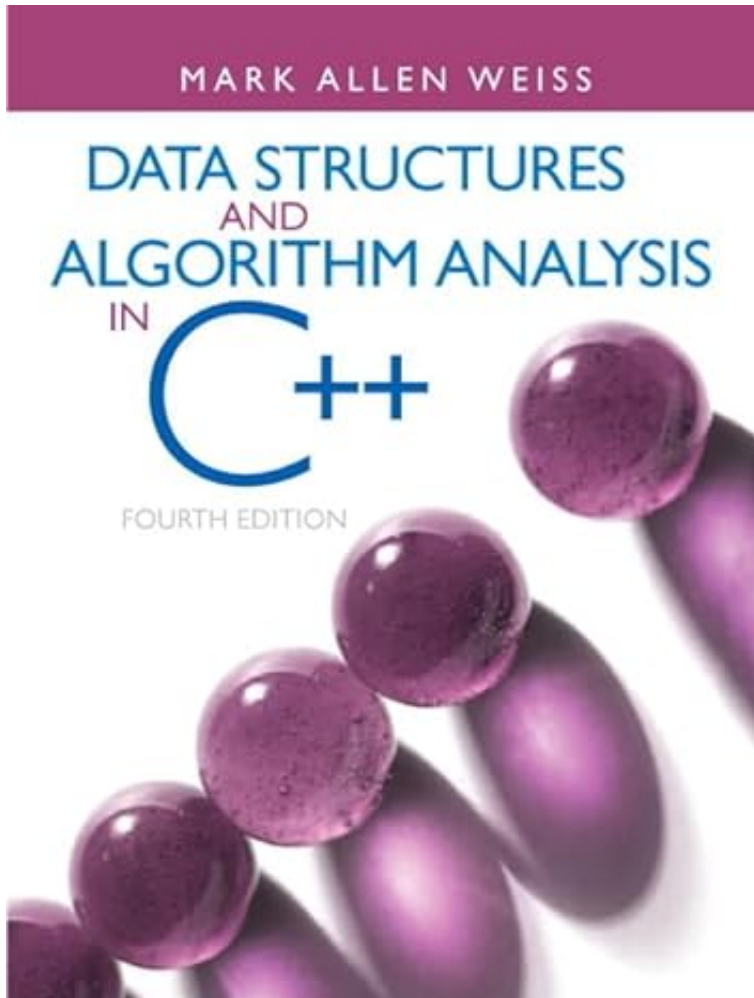
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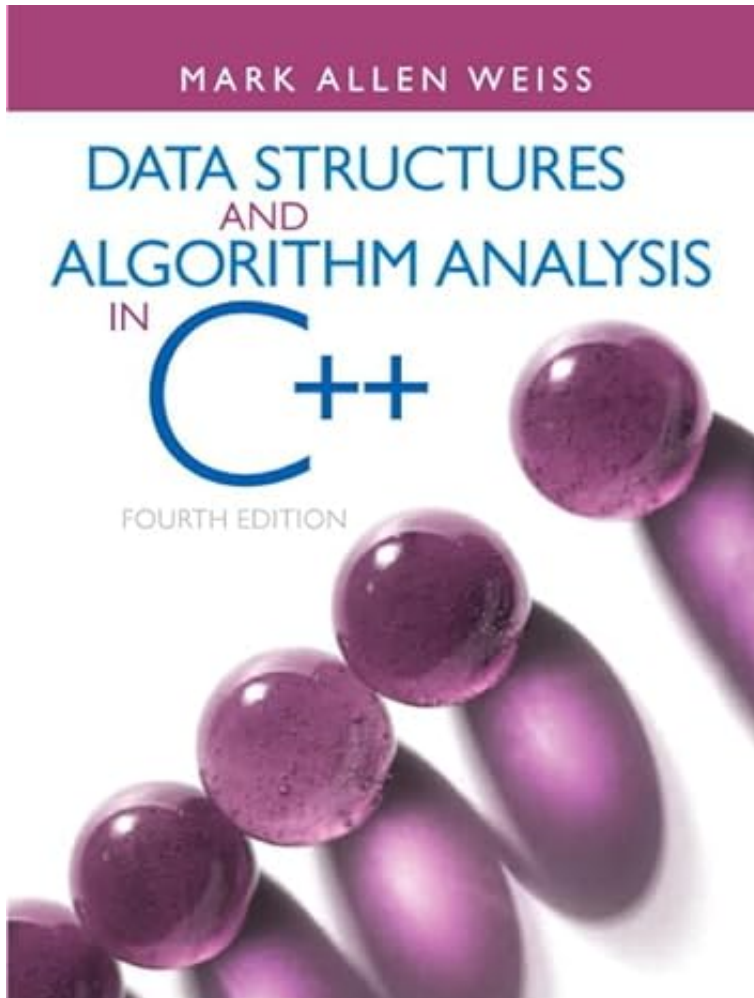


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# What is a Data Structure?

*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

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*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*

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# 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

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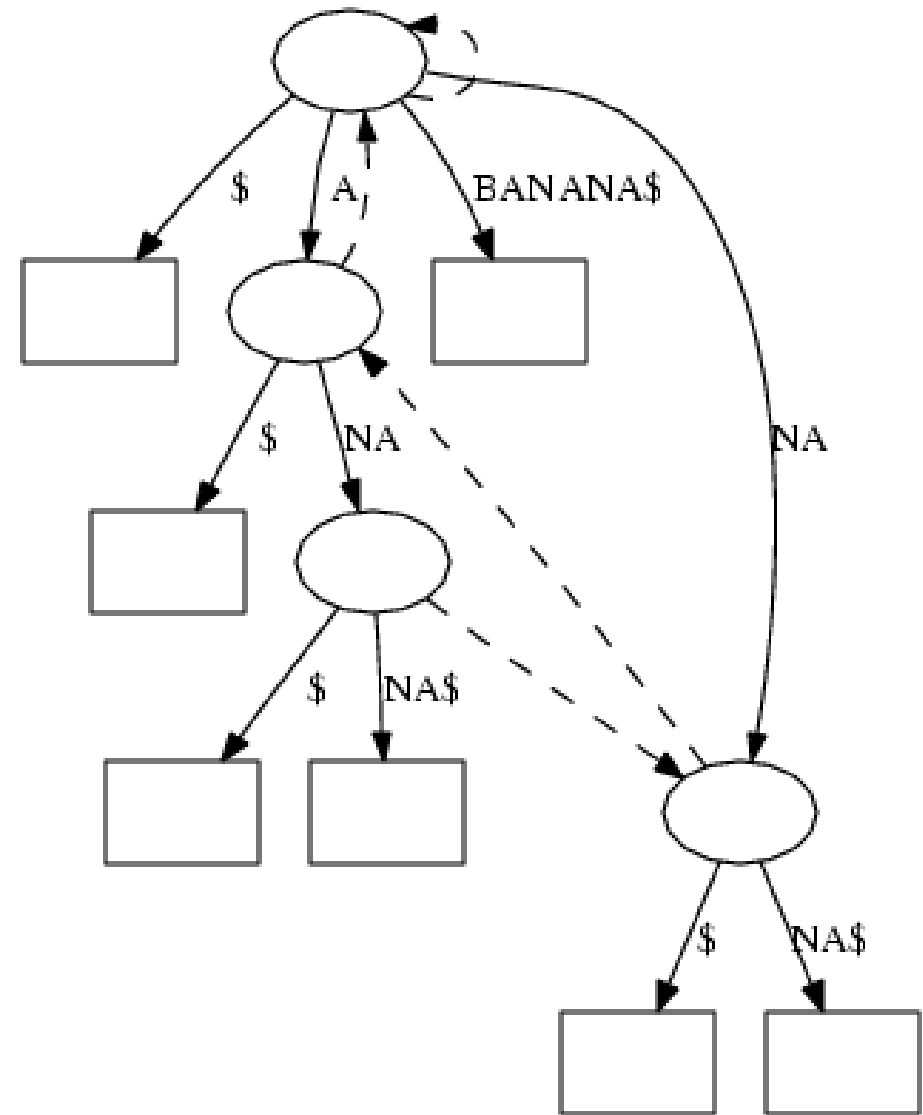
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*Thou shall not re-implement common data structures*

# Outline

1. Course structure
2. **Example of Using DSA**
3. Sophisticated Program
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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

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# Code for sort

```
#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++];
    }
}
```



```
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 ( $\sim 20$  lines of code)
- Uses a simple array
- Difficult to see what is going on
- On 100 000 inputs it takes 10 seconds to run

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# Using Data Structures and algorithms

```
#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

```
#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
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Data structure version is

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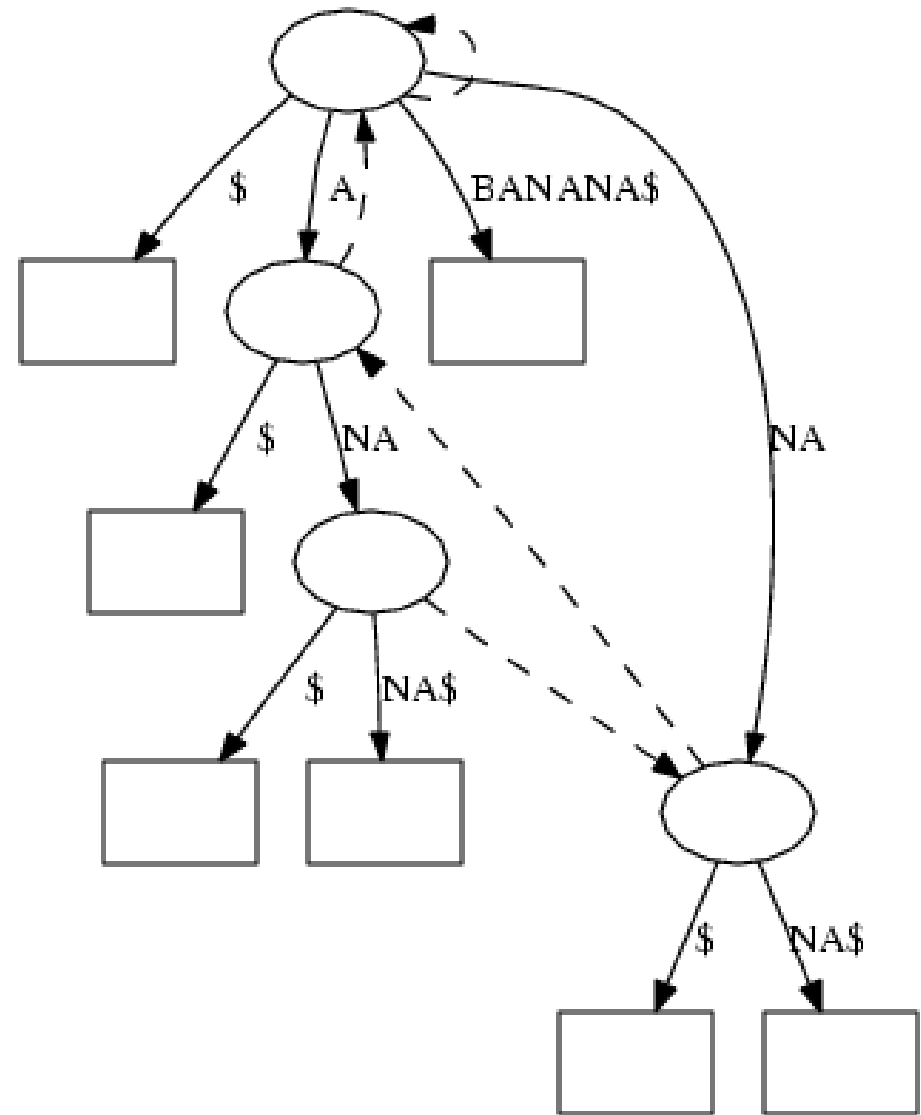
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# Sophisticated Programs

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# countWords

```
#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 than 10 times as much code that runs in less than 10 times as long*

- Probably possible, but certainly not easy



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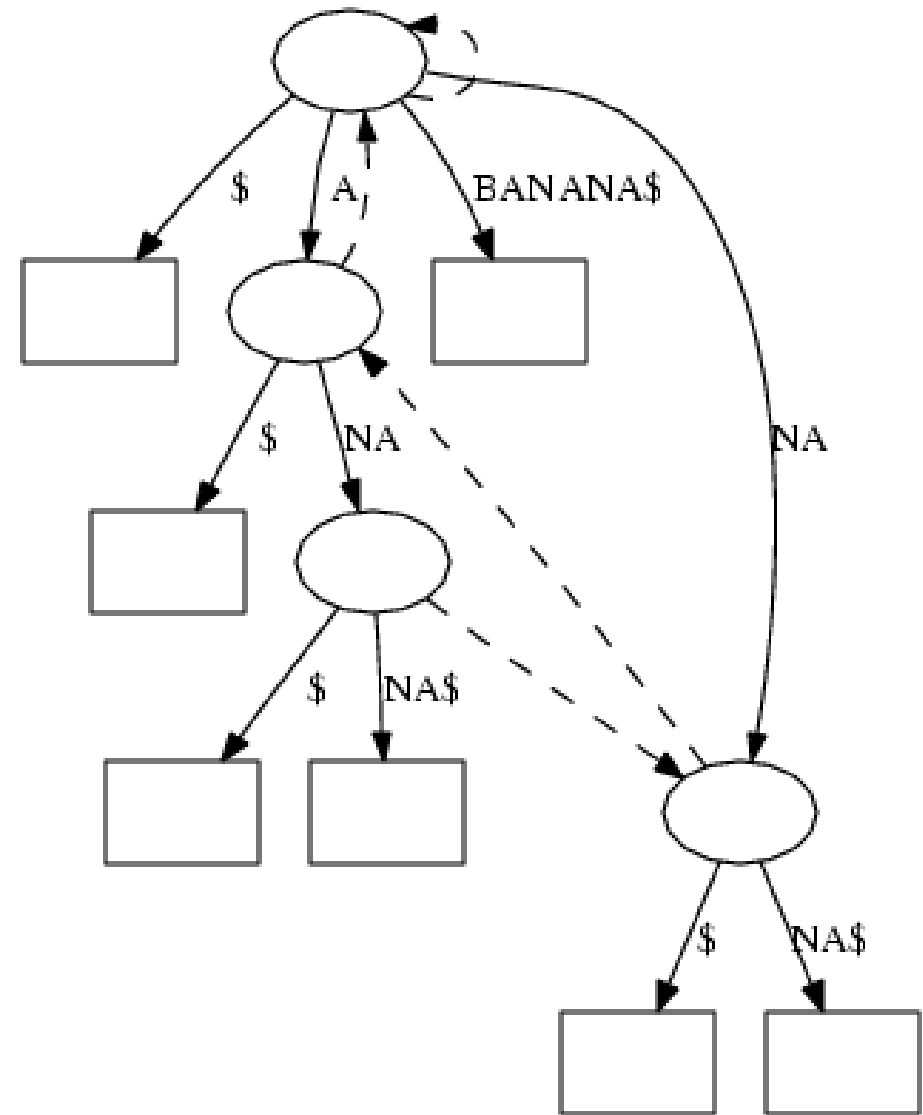
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# Sequencing and Assembly

A T A C C A C C A T G C C T C C T T G C T C C A A T A T T A A T T C A A G G C G

# Sequencing and Assembly

ATACCAACCATGCCTCCTTTGCTCCAATATTAAATTCAGGCG  
ATACCAACCATGCCTCCTTTGCTCCAATATTAAATTCAGGCG  
ATACCAACCATGCCTCCTTTGCTCCAATATTAAATTCAGGCG  
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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

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ATACC

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

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TGCCT	AATAT	CCTCC	AGGCG	ATACC	ACCAT
CTCCT	CCTTG	ATGCC	GCTCC	TGCCT	TTGCT
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ATACCAAC

TTGCT	TACCA	CAAGG	TTAAT	TTCAA	TCCTT
TGCCT	AATAT	CCTCC	AGGCG	ATACC	ACCAT
CTCCT	CCTTG	ATGCC	GCTCC	TGCCT	TTGCT
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ATACCAACCA

TTGCT	TACCA	CAAGG	TTAAT	TTCAA	TCCTT
TGCCT	AATAT	CCTCC	AGGCG	ATACC	ACCAT
CTCCT	CCTTG	ATGCC	GCTCC	TGCCT	TTGCT
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ATACCAACCAT

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



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ATACCAACCATGCC

TTGCT	TACCA	CAAGG	TTAAT	TTCAA	TCCTT
TGCCT	AATAT	CCTCC	AGGCG	ATACC	ACCAT
CTCCT	CCTTG	ATGCC	GCTCC	TGCCT	TTGCT
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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

# Sequencing and Assembly

ATACCAACCATGCCTCCTTTGCTCCCAATATTAAATTCAGGCG  
ATACCAACCATGCCTCCTTTGCTCCCAATATTAAATTCAGGCG  
ATACCAACCATGCCTCCTTTGCTCCCAATATTAAATTCAGGCG  
ATACCAACCATGCCTCCTTTGCTCCCAATATTAAATTCAGGCG  
ATACCAACCATGCCTCCTTTGCTCCCAATATTAAATTCAGGCG

ATACCAACCATGCCTCC

TTGCT	TACCA	CAAGG	TTAAT	TTCAA	TCCTT
TGCCT	AATAT	CCTCC	AGGCG	ATACC	ACCAT
CTCCT	CCTTG	ATGCC	GCTCC	TGCCT	TTGCT
TGCTC	ACCAC	TTGCT	AATAT	CAAGG	TGCCT
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 ATACCAACCATGCCTCCTTTGCTCCCAATATTAAATTCAGGCG  
 ATACCAACCATGCCTCCTTTGCTCCCAATATTAAATTCAGGCG  
 ATACCAACCATGCCTCCTTTGCTCCCAATATTAAATTCAGGCG  
 ATACCAACCATGCCTCCTTTGCTCCCAATATTAAATTCAGGCG

ATACCAACCATGCCTCCTT

TTGCT	TACCA	CAAGG	TTAAT	TTCAA	TCCTT
TGCCT	AATAT	CCTCC	AGGCG	ATACC	ACCAT
CTCCT	CCTTG	ATGCC	GCTCC	TGCCT	TTGCT
TGCTC	ACCAC	TTGCT	AATAT	CAAGG	TGCCT
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ATACCAACCATGCCTCCTTT

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

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ATACCAACCATGCTCCTTTGCTCCCAATATTAAATTC AAGGCG  
ATACCAACCATGCTCCTTTGCTCCCAATATTAAATTC AAGGCG  
ATACCAACCATGCTCCTTTGCTCCCAATATTAAATTC AAGGCG  
ATACCAACCATGCTCCTTTGCTCCCAATATTAAATTC AAGGCG  
ATACCAACCATGCTCCTTTGCTCCCAATATTAAATTC AAGGCG

ATACCAACCATGCTCCTTTG

TTGCT	TACCA	CAAGG	TTAAT	TTCAA	TCCTT
TGCCT	AATAT	CCTCC	AGGCG	ATACC	ACCAT
CTCCT	CCTTG	ATGCC	GCTCC	TGCCT	TTGCT
TGCTC	ACCAC	TTGCT	AATAT	CAAGG	TGCCT
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ATACCAACCATGCCTCCTTTGCT

TTGCT	TACCA	CAAGG	TTAAT	TTCAA	TCCTT
TGCCT	AATAT	CCTCC	AGGCG	ATACC	ACCAT
CTCCT	CCTTG	ATGCC	GCTCC	TGCCT	TTGCT
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ATACCAACCATGCCTCCTTTGCTCCCAATATTAAATTC AAGGCG

ATACCAACCATGCCTCCTTTGCTC

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



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ATACCAACCATGCCTCCTTTGCTCCCAATATTAAATTCAGGCG  
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ATACCAACCATGCCTCCTTTGCTCC

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

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A T A C C A C C A T G C C T C C T T G C T C C A A T A T T A A T T C A A G G C G  
A T A C C A C C A T G C C T C C T T G C T C C A A T A T T A A T T C A A G G C G  
A T A C C A C C A T G C C T C C T T G C T C C A A T A T T A A T T C A A G G C G  
A T A C C A C C A T G C C T C C T T G C T C C A A T A T T A A T T C A A G G C G  
A T A C C A C C A T G C C T C C T T G C T C C A A T A T T A A T T C A A G G C G

A T A C C A C C A T G C C T C C T T G C T C C A

TTGCT	TACCA	CAAGG	TTAAT	TTCAA	TCCTT
TGCCT	AATAT	CCTCC	AGGCG	ATACC	ACCAT
CTCCT	CCTTG	ATGCC	GCTCC	TGCCT	TTGCT
TGCTC	ACCAC	TTGCT	AATAT	CAAGG	TGCCT
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ATACCAACCATGCCTCCTTTGCTCCCAATATTAAATTCAGGCG  
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ATACCAACCATGCCTCCTTTGCTCCCAATAT

TTGCT	TACCA	CAAGG	TTAAT	TTCAA	TCCTT
TGCCT	AATAT	CCTCC	AGGCG	ATACC	ACCAT
CTCCT	CCTTG	ATGCC	GCTCC	TGCCT	TTGCT
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ATACCAACCATGCCTCCTTTGCTCCCAATATTAAATTCAGGCG  
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ATACCAACCATGCCTCCTTTGCTCCCAATATTAA

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

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A T A C C A C C A T G C C T C C T T G C T C C A A T A T T A A T T C A A G G C G  
A T A C C A C C A T G C C T C C T T G C T C C A A T A T T A A T T C A A G G C G  
A T A C C A C C A T G C C T C C T T G C T C C A A T A T T A A T T C A A G G C G  
A T A C C A C C A T G C C T C C T T G C T C C A A T A T T A A T T C A A G G C G  
A T A C C A C C A T G C C T C C T T G C T C C A A T A T T A A T T C A A G G C G

A T A C C A C C A T G C C T C C T T G C T C C A A T A T T A A T

TTGCT	TACCA	CAAGG	TTAAT	TTCAA	TCCTT
TGCCT	AATAT	CCTCC	AGGCG	ATACC	ACCAT
CTCCT	CCTTG	ATGCC	GCTCC	TGCCT	TTGCT
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A T A C C A C C A T G C C T C C T T G C T C C A A T A T T A A T T C A A G G C G  
A T A C C A C C A T G C C T C C T T G C T C C A A T A T T A A T T C A A G G C G  
A T A C C A C C A T G C C T C C T T G C T C C A A T A T T A A T T C A A G G C G  
A T A C C A C C A T G C C T C C T T G C T C C A A T A T T A A T T C A A G G C G  
A T A C C A C C A T G C C T C C T T G C T C C A A T A T T A A T T C A A G G C G

A T A C C A C C A T G C C T C C T T G C T C C A A T A T T A A T T C

TTGCT	TACCA	CAAGG	TTAAT	TTCAA	TCCTT
TGCCT	AATAT	CCTCC	AGGCG	ATACC	ACCAT
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TACCA	CACCA	CCTTG	CTCCA	TATTA	AATTC

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A T A C C A C C A T G C C T C C T T G C T C C A A T A T T A A T T C A A G G C G  
A T A C C A C C A T G C C T C C T T G C T C C A A T A T T A A T T C A A G G C G  
A T A C C A C C A T G C C T C C T T G C T C C A A T A T T A A T T C A A G G C G  
A T A C C A C C A T G C C T C C T T G C T C C A A T A T T A A T T C A A G G C G  
A T A C C A C C A T G C C T C C T T G C T C C A A T A T T A A T T C A A G G C G

A T A C C A C C A T G C C T C C T T G C T C C A A T A T T A A T T C A A

TTGCT	TACCA	CAAGG	TTAAT	TTCAA	TCCTT
TGCCT	AATAT	CCTCC	AGGCG	ATACC	ACCAT
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A T A C C A C C A T G C C T C C T T G C T C C A A T A T T A A T T C A A G G C G  
A T A C C A C C A T G C C T C C T T G C T C C A A T A T T A A T T C A A G G C G  
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A T A C C A C C A T G C C T C C T T G C T C C A A T A T T A A T T C A A G G

TTGCT	TACCA	CAAGG	TTAAT	TTCAA	TCCTT
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A T A C C A C C A T G C C T C C T T G C T C C A A T A T T A A T T C A A G G C G  
A T A C C A C C A T G C C T C C T T G C T C C A A T A T T A A T T C A A G G C G  
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A T A C C A C C A T G C C T C C T T G C T C C A A T A T T A A T T C A A G G C G  
A T A C C A C C A T G C C T C C T T G C T C C A A T A T T A A T T C A A G G C G

A T A C C A C C A T G C C T C C T T G C T C C A A T A T T A A T T C A A G G C G

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?

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# Repeats

- The difficulty of assembly is caused by repeats

A T A C C A C C A T G C C T C C T T G C T C C A A T C C A C C A T C A A G G C G

- How many repeats are there in the human genome?
- This is an important question for developing new sequencing technologies

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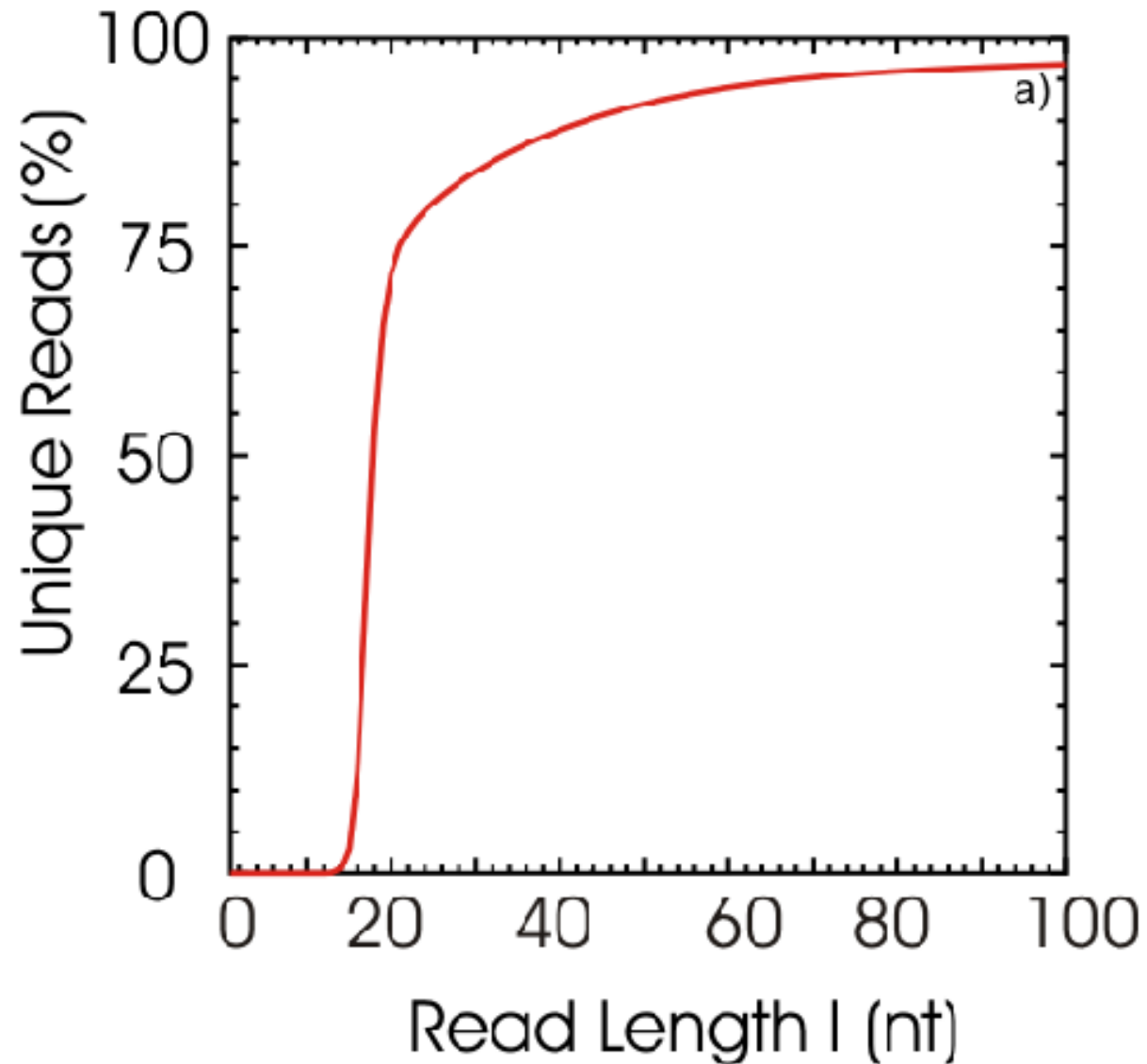
# Repeats

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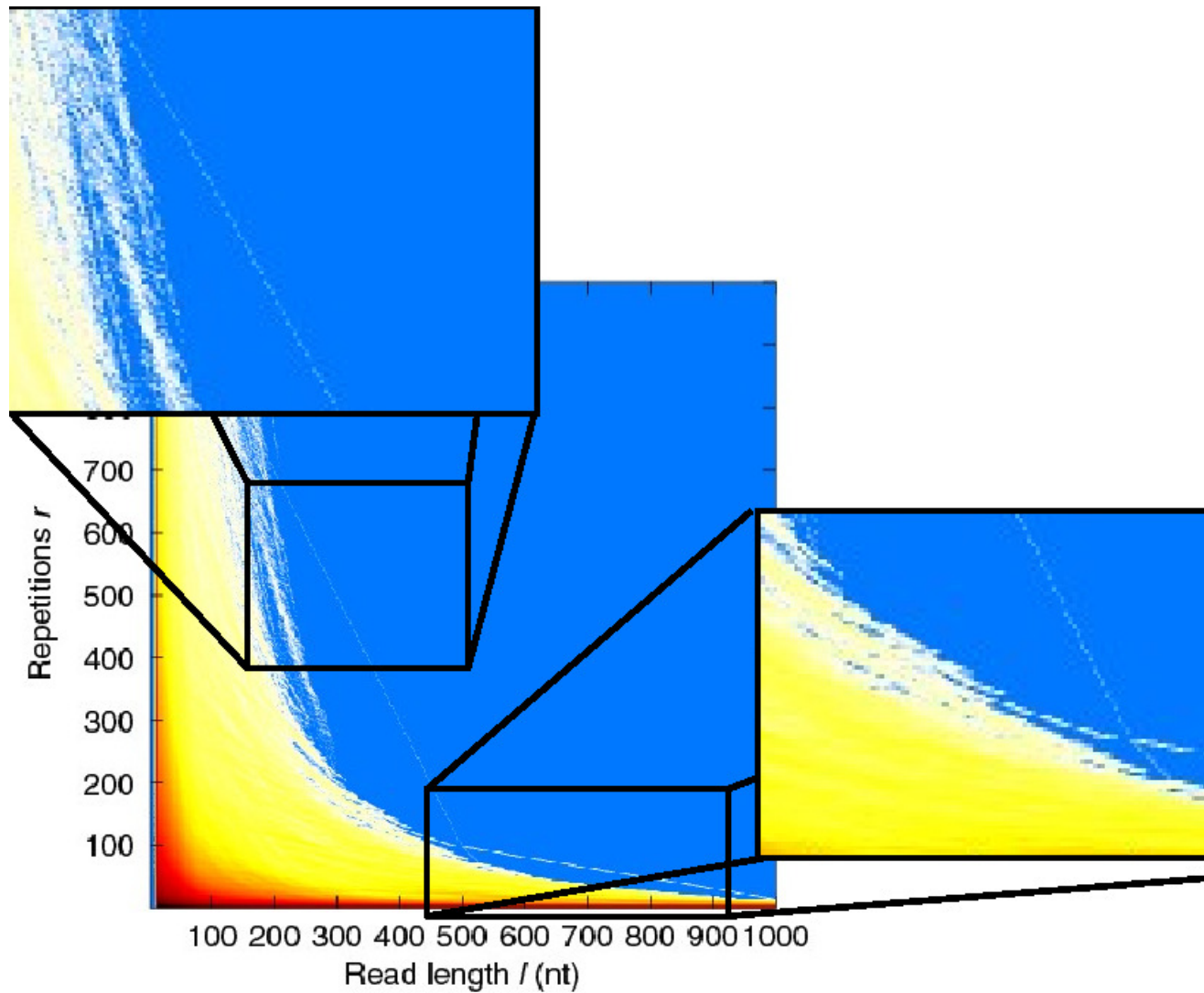
A T A C C A C C A T G C C T C C T T G C T C C A A T C C A C C A T C A A G G C G

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# 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
- Used state-of-the-art suffix arrays
- Smart algorithms allow you to do things which you cannot do otherwise

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# 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
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