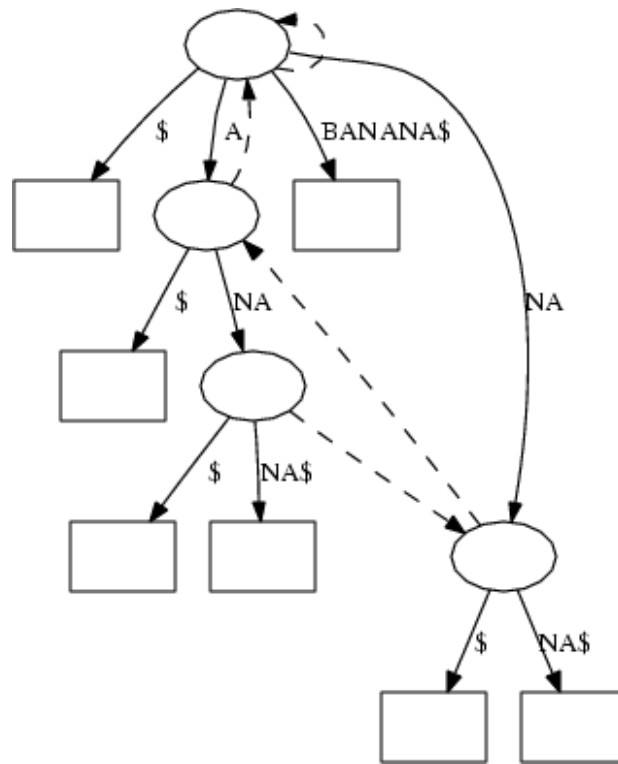


Algorithms and Analysis

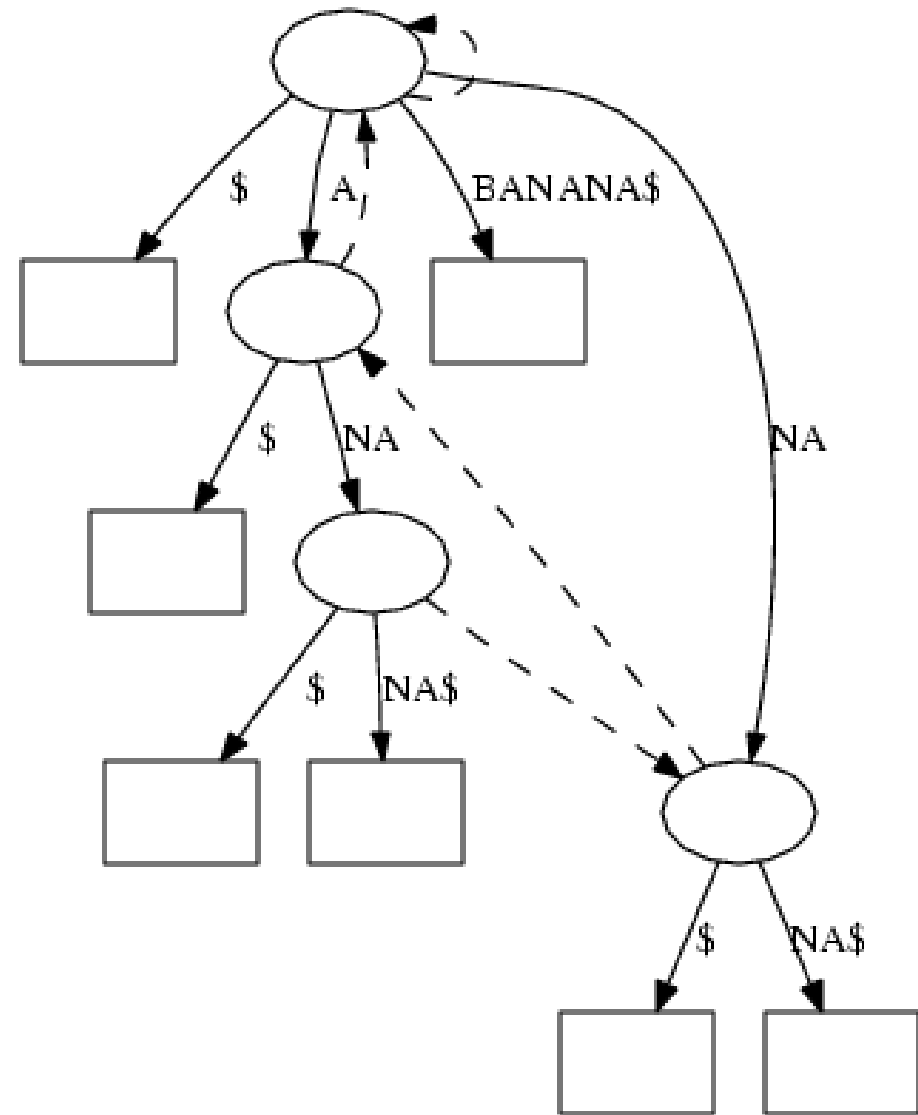
Lesson 1: *Use Data Structures and Algorithms!*



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



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- Taught by Dr Daniela Mihai and me (Adam Prügel-Bennett)
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Course Structure

- 30ish lectures

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- 4 labs (worth 10%)

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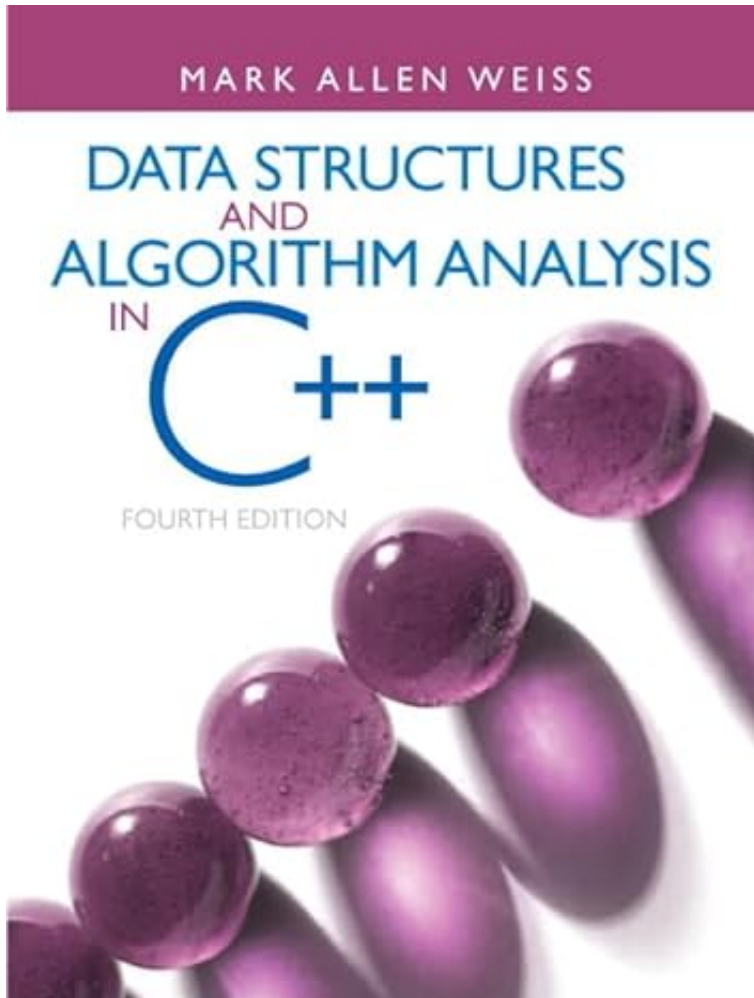
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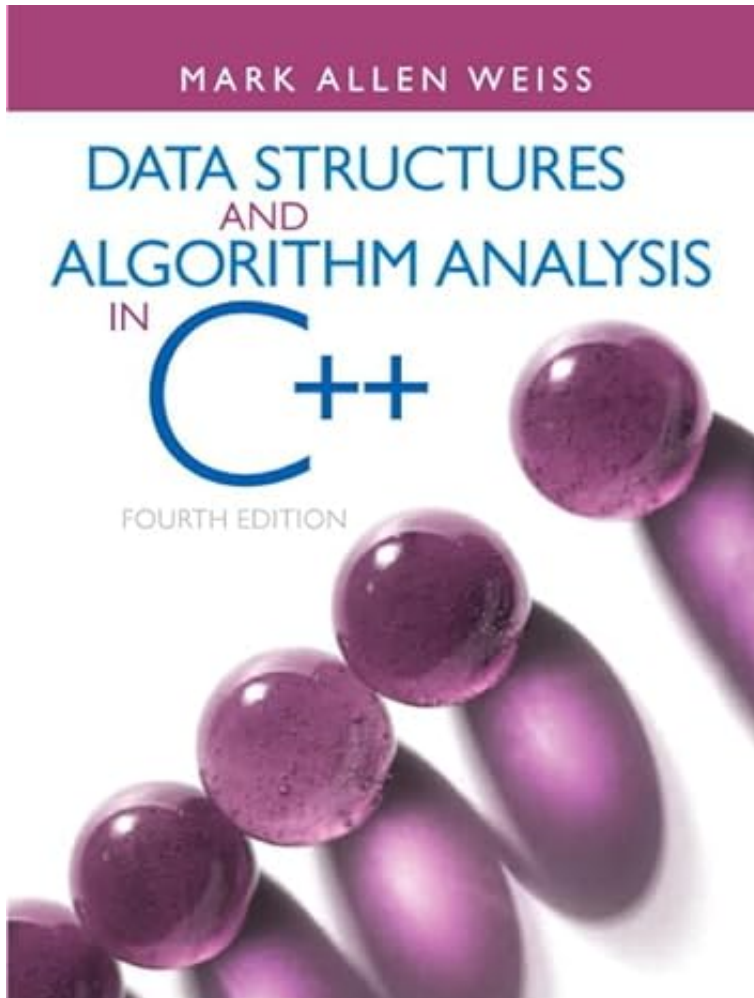
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- Final exam (worth 50%?)

Recommended Course Text



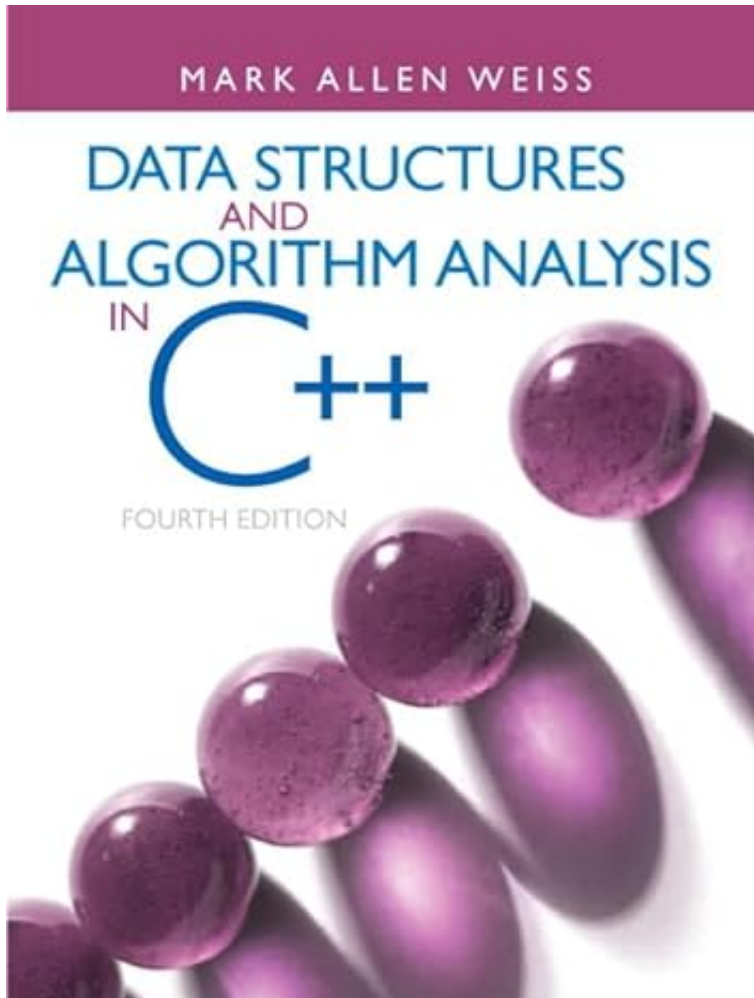
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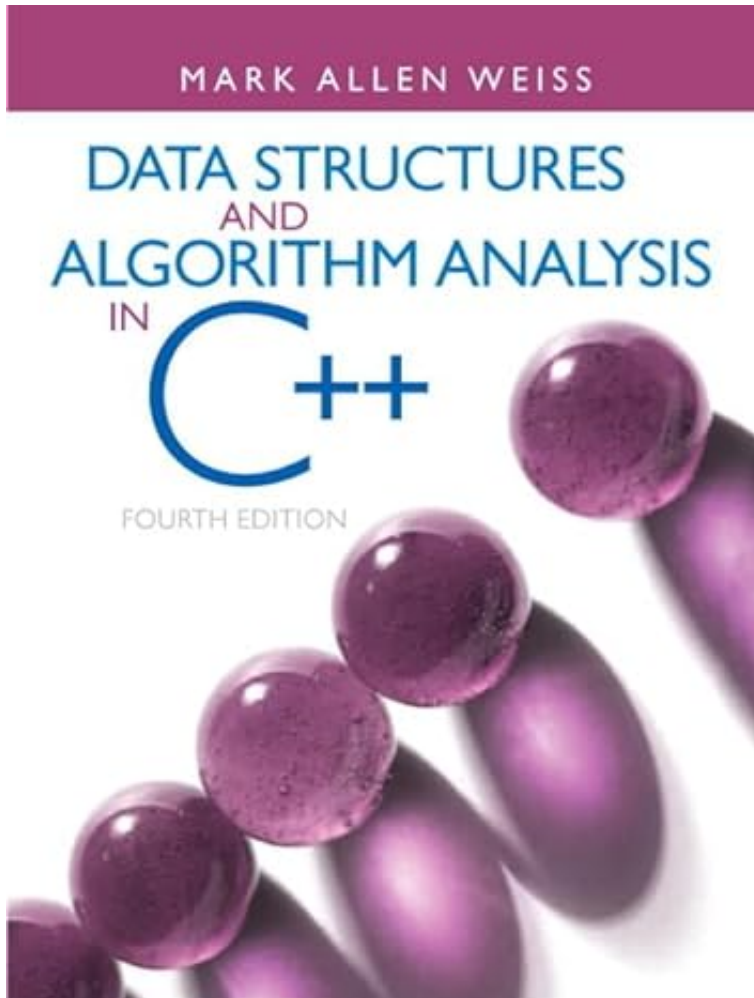
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What is a Data Structure?

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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- Well defined and generic
- Guarantees on performance

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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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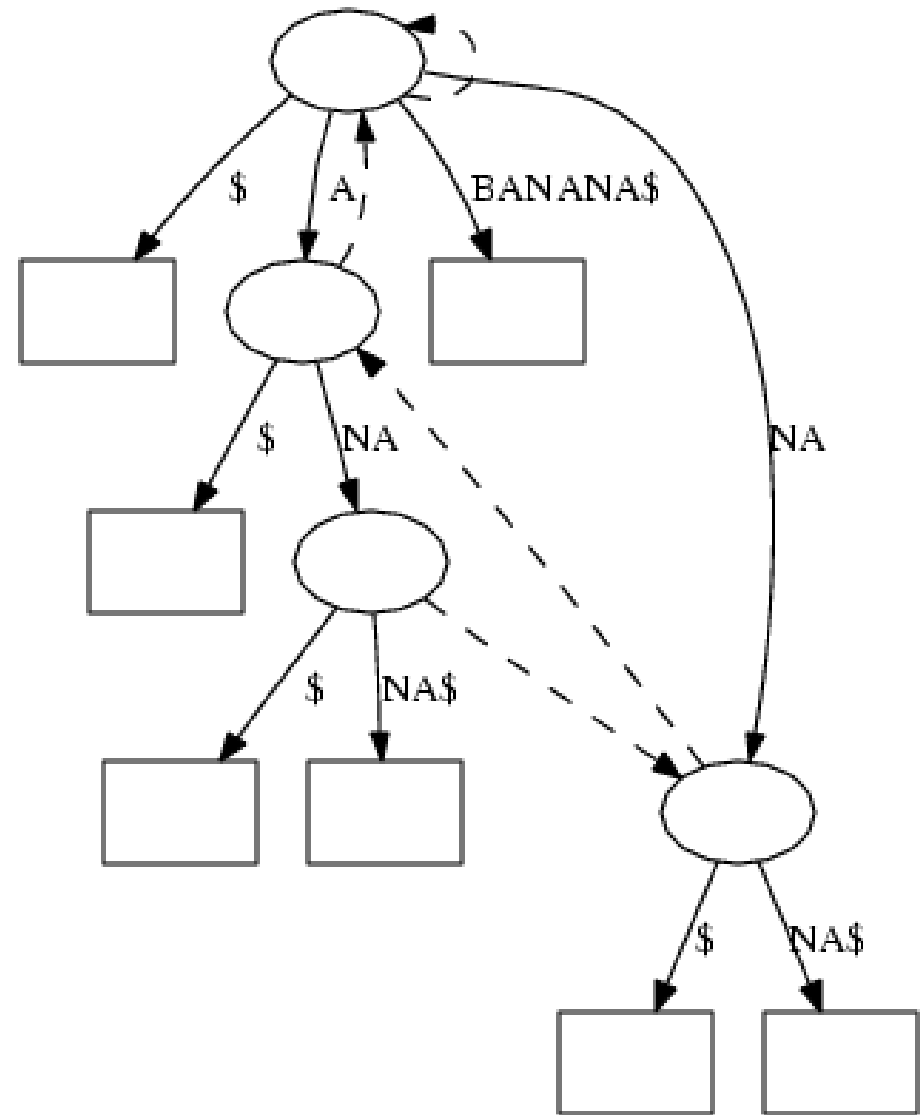
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Thou shall not re-implement common data structures

Outline

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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 (~ 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
- On 100 000 inputs takes 10ms to run

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Data structure version is

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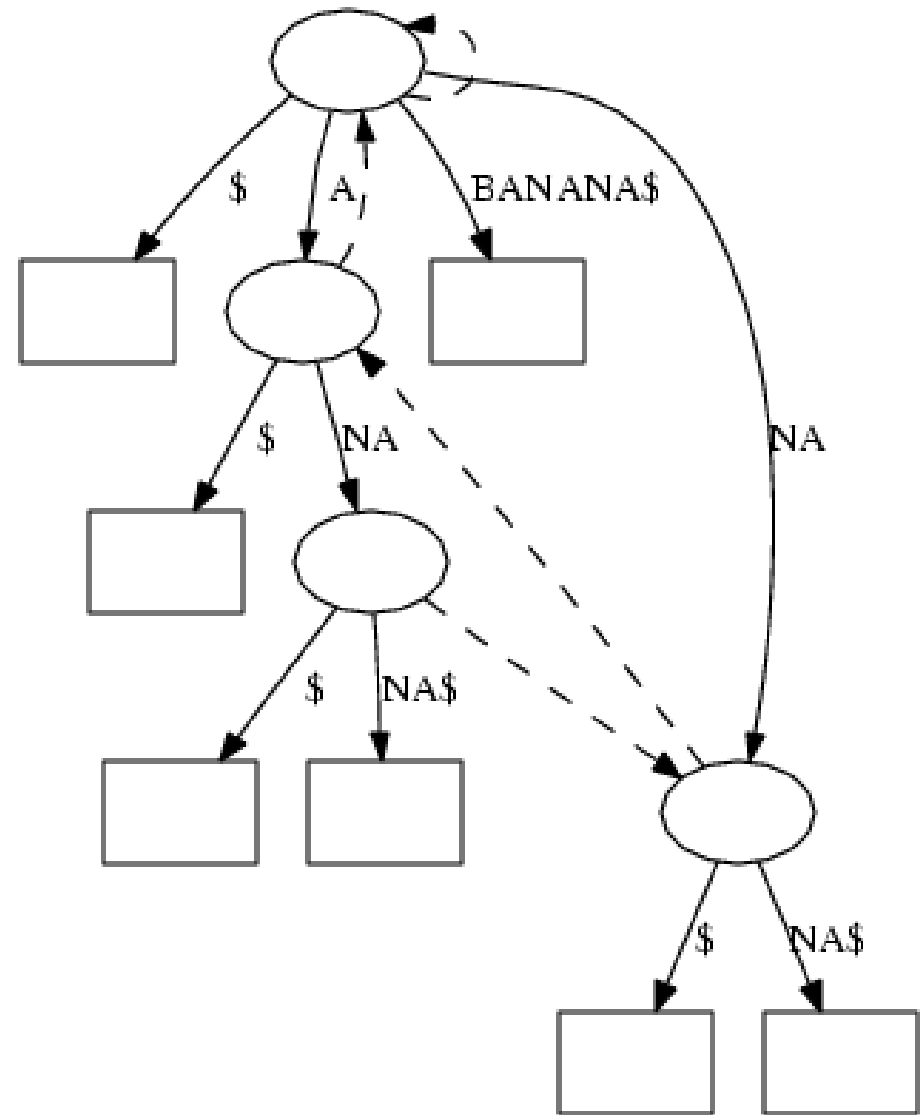
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Sophisticated Programs

- 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
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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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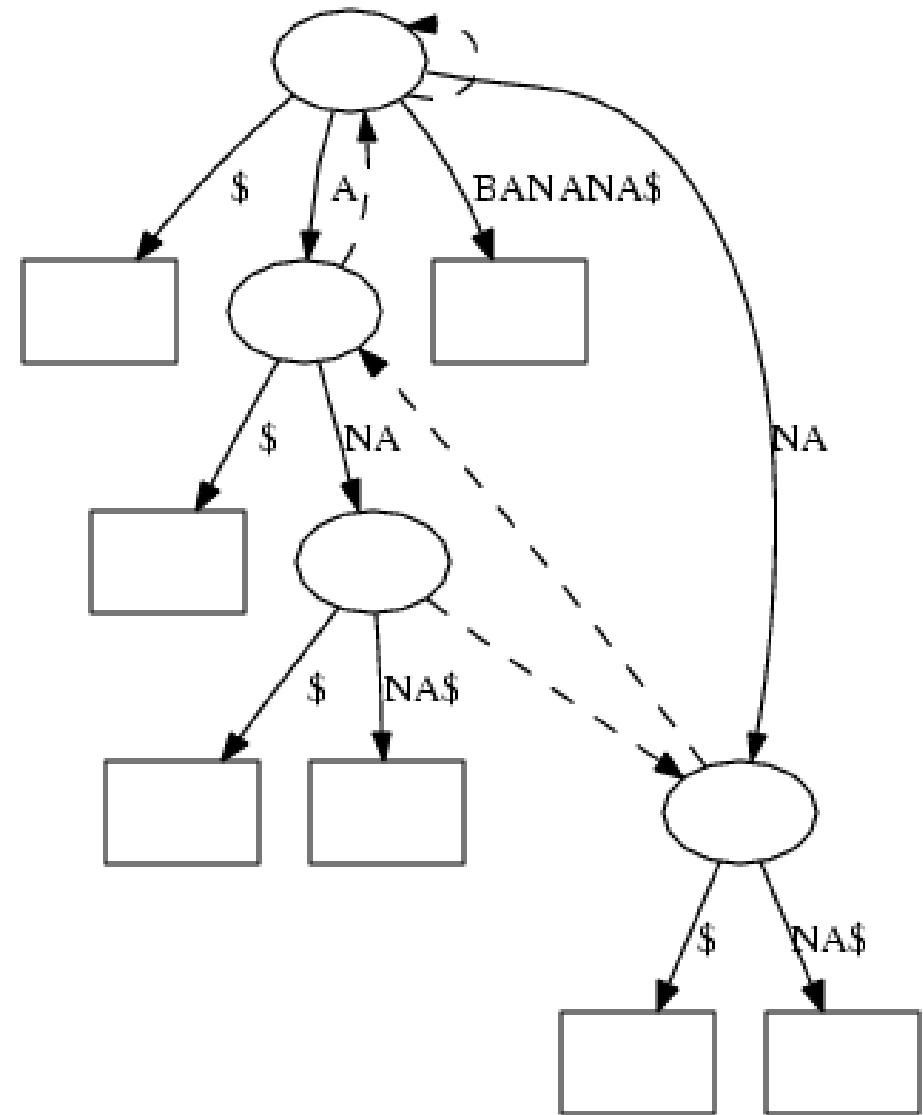
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DNA Sequencing

- In modern whole shotgun genome sequencing the full genome is broken into small pieces
- The pieces are then read by a sequencing machine
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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

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

Sequencing and Assembly

ATACCAACCATGCCTCCTTTGCTCCCAATATTAAATTCAGGCG
ATACCAACCATGCCTCCTTTGCTCCCAATATTAAATTCAGGCG
ATACCAACCATGCCTCCTTTGCTCCCAATATTAAATTCAGGCG
ATACCAACCATGCCTCCTTTGCTCCCAATATTAAATTCAGGCG
ATACCAACCATGCCTCCTTTGCTCCCAATATTAAATTCAGGCG

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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ATACCAACCATGCCTCCTTTGCTCCCAATATTAAATTC AAGGCG
ATACCAACCATGCCTCCTTTGCTCCCAATATTAAATTC AAGGCG

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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ATACCAACCATGCCTCCTTTGCTCCCAATATTAAATTCAGGCG
ATACCAACCATGCCTCCTTTGCTCCCAATATTAAATTCAGGCG

ATACCA

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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ATACCAACCATGCCTCCTTTGCTCCCAATATTAAATTC AAGGCG
ATACCAACCATGCCTCCTTTGCTCCCAATATTAAATTC AAGGCG

ATACCAAC

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

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ATACCAACCATGCCTCCTTTGCTCCCAATATTAAATTCAGGCG
ATACCAACCATGCCTCCTTTGCTCCCAATATTAAATTCAGGCG

ATACCAACCA

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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ATACCAACCATGCCTCCTTTGCTCCCAATATTAAATTCAGGCG
ATACCAACCATGCCTCCTTTGCTCCCAATATTAAATTCAGGCG

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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ATACCAACCATGCCTCCTTTGCTCCCAATATTAAATTCAGGCG
ATACCAACCATGCCTCCTTTGCTCCCAATATTAAATTCAGGCG

ATACCAACCATGCC

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

ATACCAACCATGCCTCCTTTGCTCCCAATATTAAATTC AAGGCG
ATACCAACCATGCCTCCTTTGCTCCCAATATTAAATTC AAGGCG
ATACCAACCATGCCTCCTTTGCTCCCAATATTAAATTC AAGGCG
ATACCAACCATGCCTCCTTTGCTCCCAATATTAAATTC AAGGCG
ATACCAACCATGCCTCCTTTGCTCCCAATATTAAATTC AAGGCG

ATACCAACCATGCCT

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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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
TACCA	CACCA	CCTTG	CTCCA	TATTA	AATTC

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ATACCAACCATGCCTCCTTTGCTCCCAATATTAAATTCAGGCG
ATACCAACCATGCCTCCTTTGCTCCCAATATTAAATTCAGGCG

ATACCAACCATGCCTCCTT

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

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
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

TTGCT	TACCA	CAAGG	TTAAT	TTCAA	TCCTT
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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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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

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ATACCAACCATGCCTCCTTTGCTCC

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

TTGCT	TACCA	CAAGG	TTAAT	TTCAA	TCCTT
TGCCT	AAAT	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
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

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
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

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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
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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

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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

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
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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

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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
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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

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)
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- 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

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- This is an important question for developing new sequencing technologies

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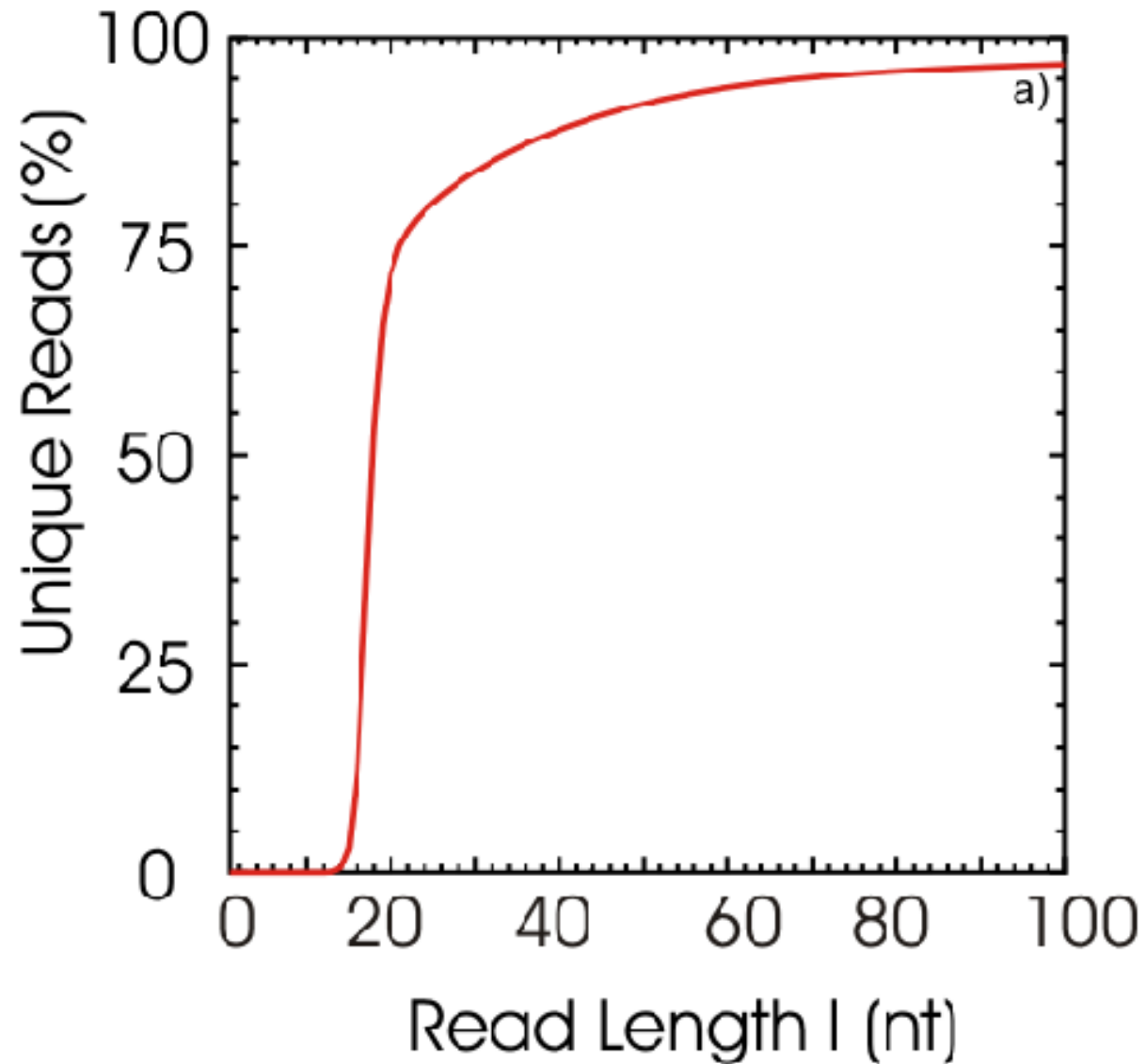
Repeats

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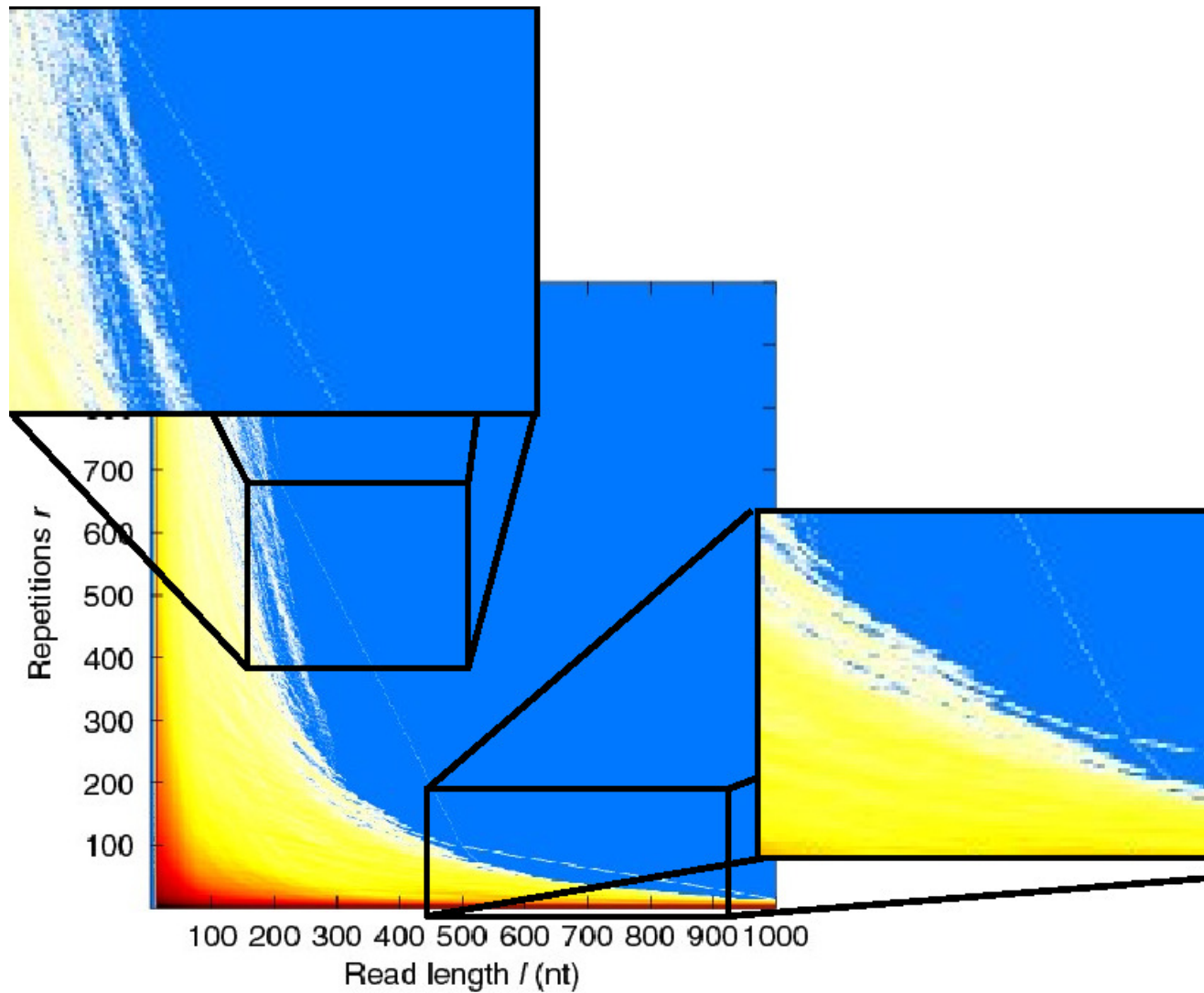
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Repeats in Human Genome



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
- The rest of this course teaches you these skills

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