# Optimization and Maintainability

David Grellscheid

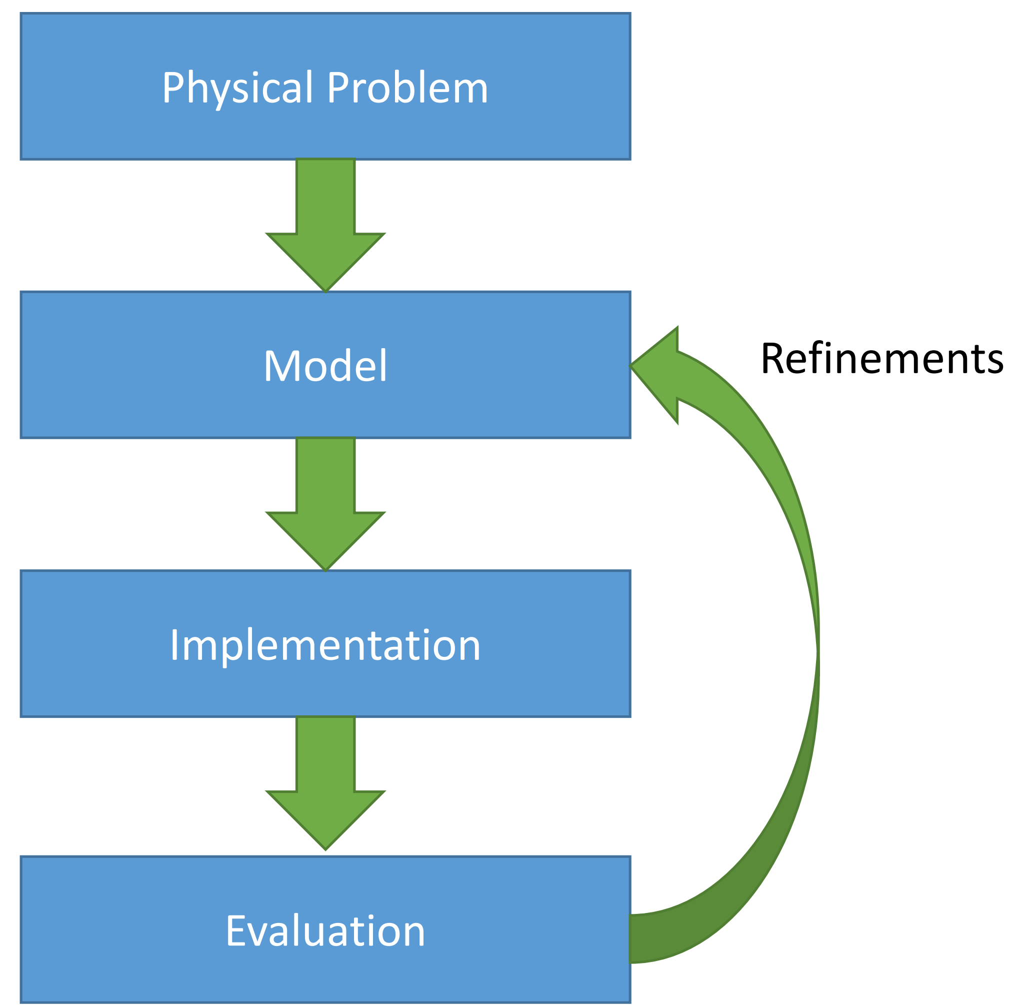
# Typical scientific workflow

Correctness is main concern

Start coding without much planning

First version that looks like it works is kept

Sub-optimal choices only noticed later on (if at all)



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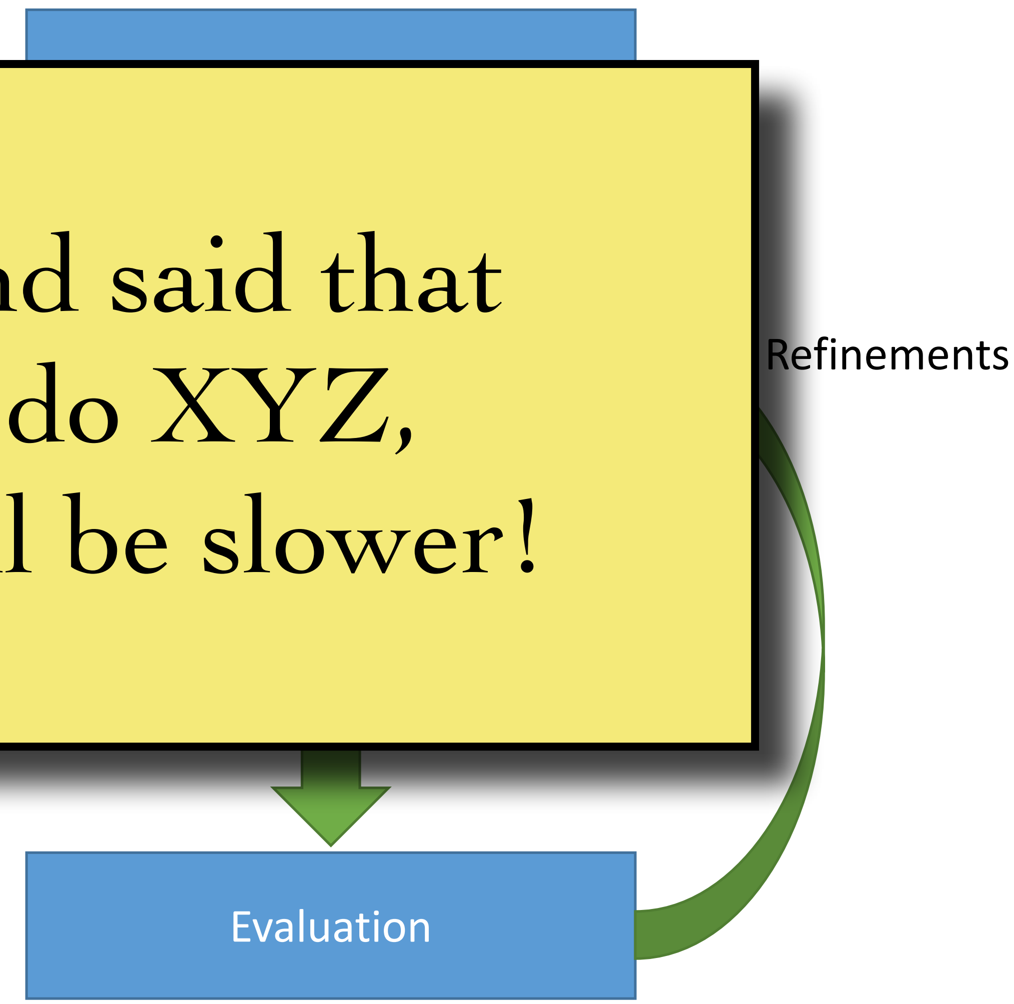


A friend of my friend said that you should never do XYZ, because the code will be slower!

# Donald Knuth, December 1974:

Programmers waste enormous amounts of time thinking about, or worrying about, the speed of noncritical parts of their programs, and these attempts at efficiency actually have a strong negative impact when debugging and maintenance are considered. We should forget about small efficiencies, say about 97% of the time: premature optimization is the root of all evil.
Yet we should not pass up our opportunities in that critical 3%.

"Structured Programming with go to Statements", Computing Surveys, Vol 6, No 4.

Runtime is not the only factor to consider,
need to think about trade off between time spent in:

development
debugging
validation
portability
runtime in your own usage
other developers' time (now/future)
total runtime for all users

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CPU time much cheaper than human time!

# Optimization points

Someone else already solved (part of) the problem:

LAPACK, BLAS
GNU scientific library
C++ Boost
Numpy, Scipy, Pandas
...

Develop googling skills, evaluate what exists.
Quality often much better than self-written attempts

# Optimization points

## Choice of programming language

Be aware of what exists

Know strengths / weaknesses

But: needs to fit rest of project

take a look at Haskell, Erlang, JS

# Optimization points

```haskell
findLongestUpTo :: Int -> (Int,Int)
findLongestUpTo mx = maximum ( map f [1 .. mx] )
   where f x = (collatzLength x,x)


collatzLength :: Int -> Int
collatzLength 1 = 1
collatzLength n = 1 + collatzLength (collatzStep n)


collatzStep :: Int -> Int
collatzStep n
   | even n    = n `div` 2
   | otherwise = 3 * n + 1
```

# Optimization points

## Program design

**First version:** understand the problems

start again

**Second version:** you know what you're doing

refactor / clean up / make reusable

**Done** :-)

# Optimization points

Algorithm / data structure choice

can get orders of magnitude in speed

Local and hardware-specific optimisations

*- later lecture -*

# Complexity basics

Much simplified, skipping formal derivation

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O(1) - constant time independent of $N$

O($N$) - linear with $N$

O($N^2$) - quadratic in $N$

# Complexity basics

Much simplified, skipping formal derivation

```
while not is_sorted(xs):
    random.shuffle(xs)
```

$O(N\, N!)$

Scaling behaviour with size $N$ of problem set:

$O(1)$ - constant time independent of $N$

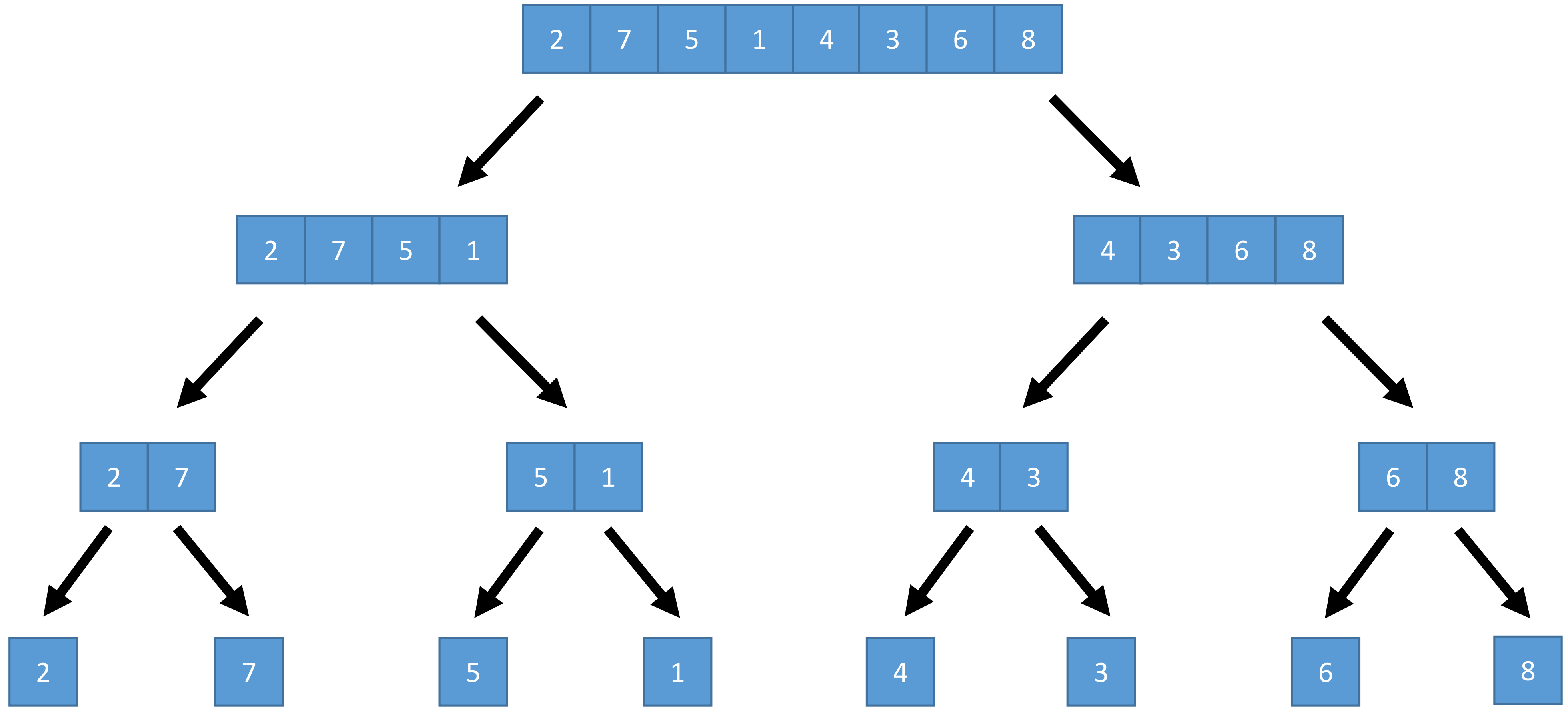
$O(N)$ - linear with $N$

$O(N^2)$ - quadratic in $N$

# Merge Sort

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 2 | 7 | 5 | 1 | 4 | 3 | 6 | 8 |

# Merge Sort



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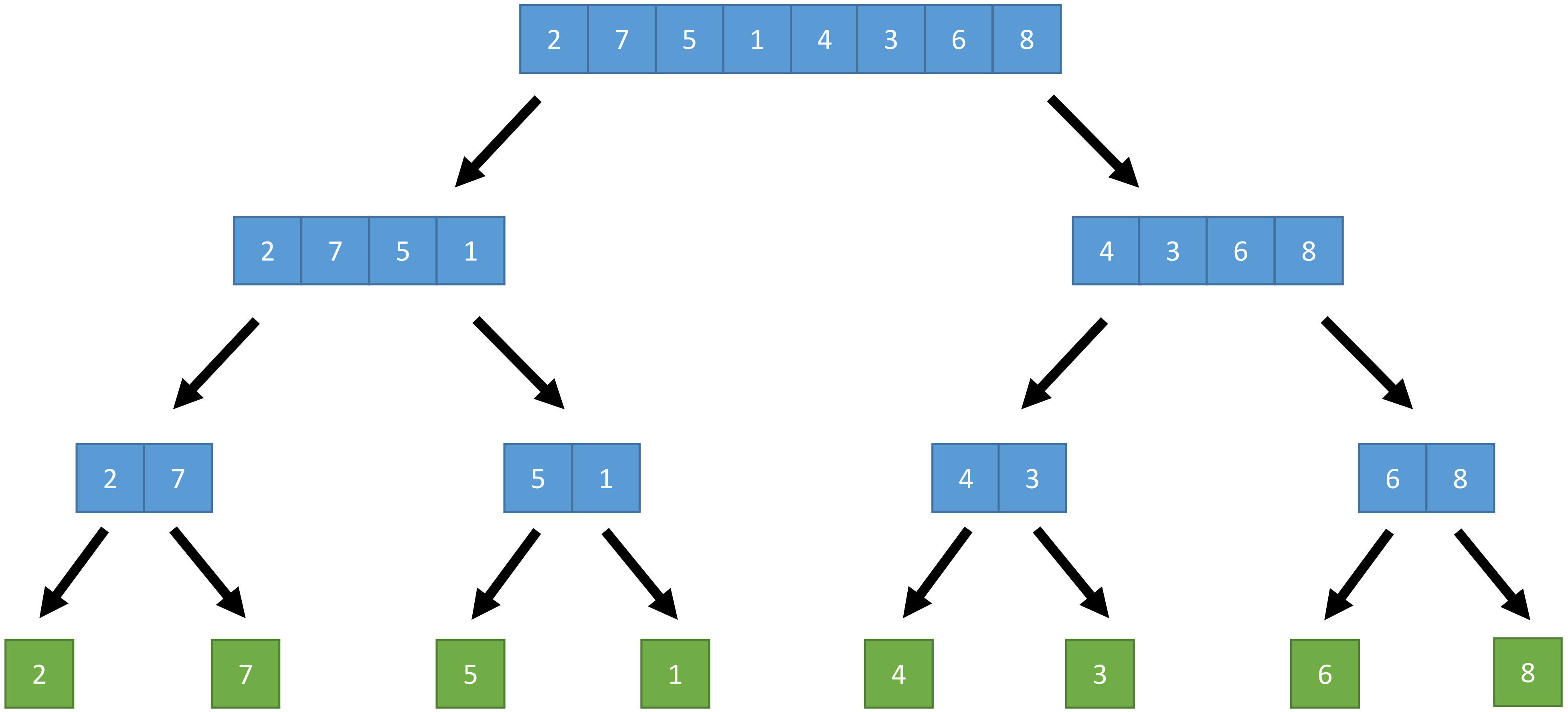

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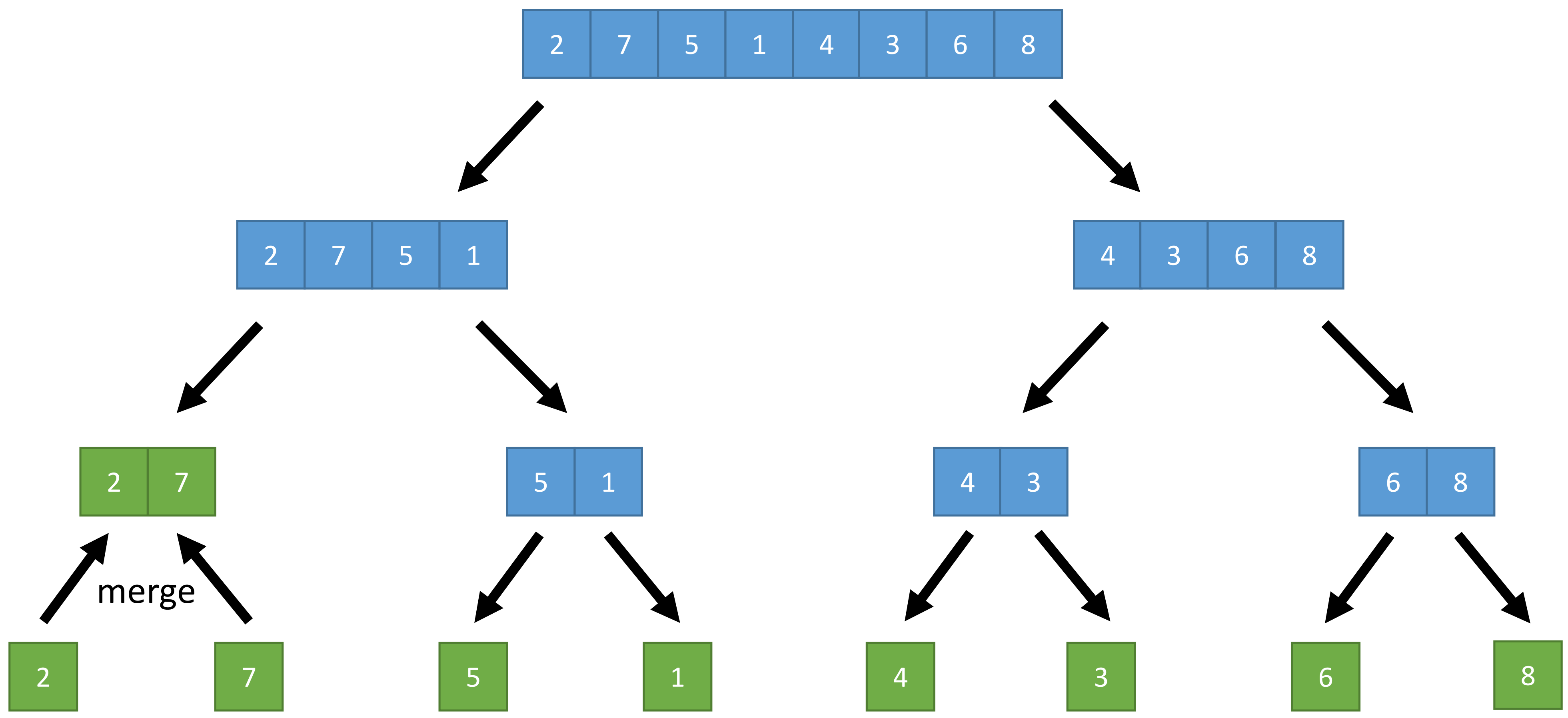

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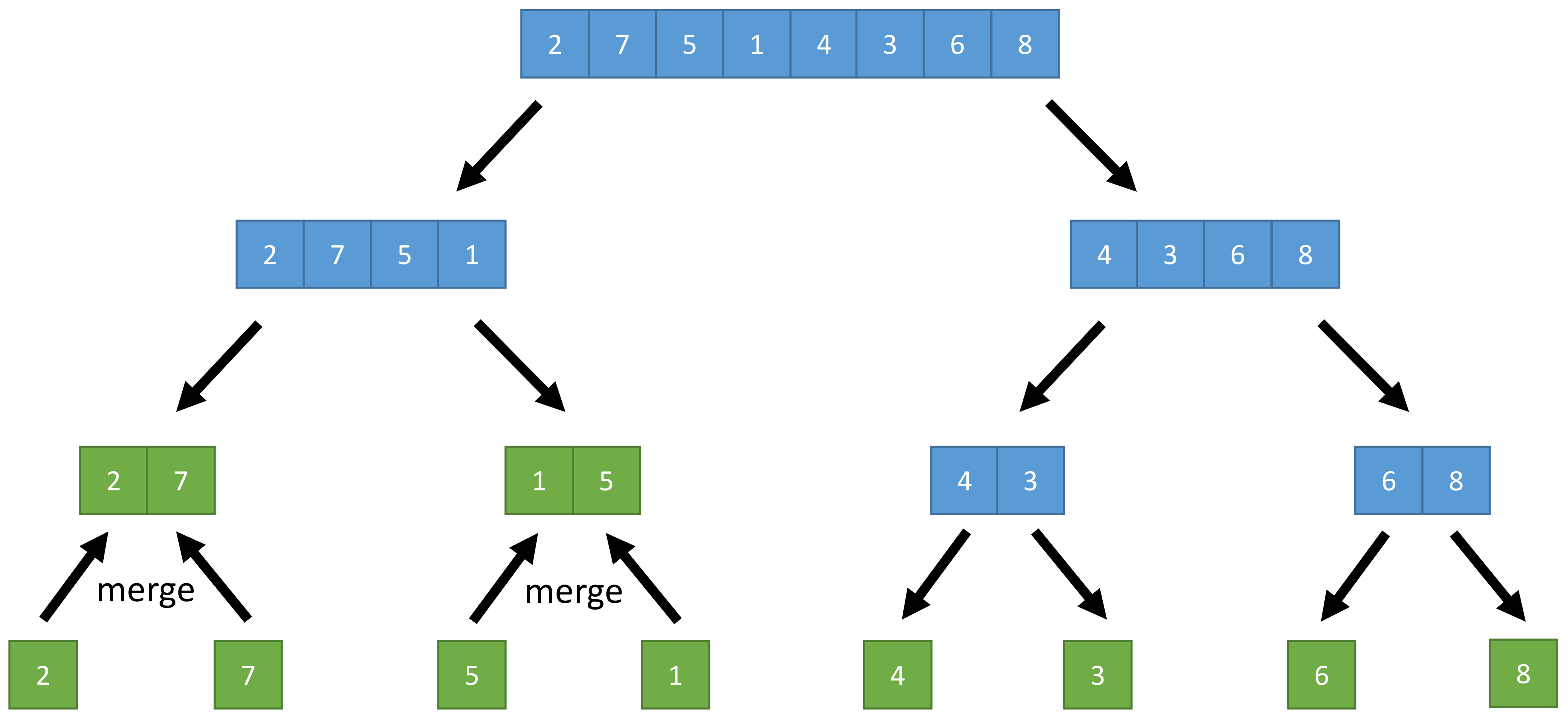

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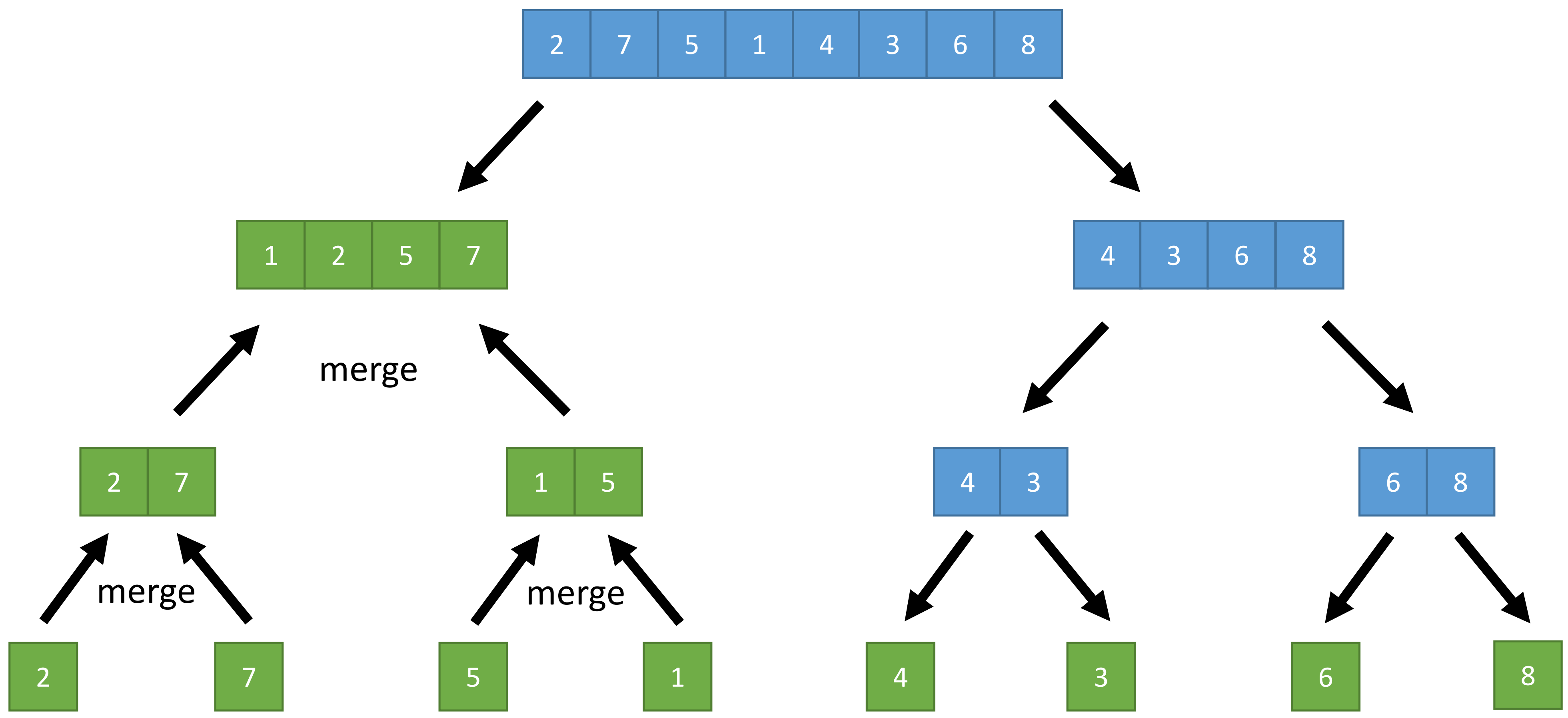

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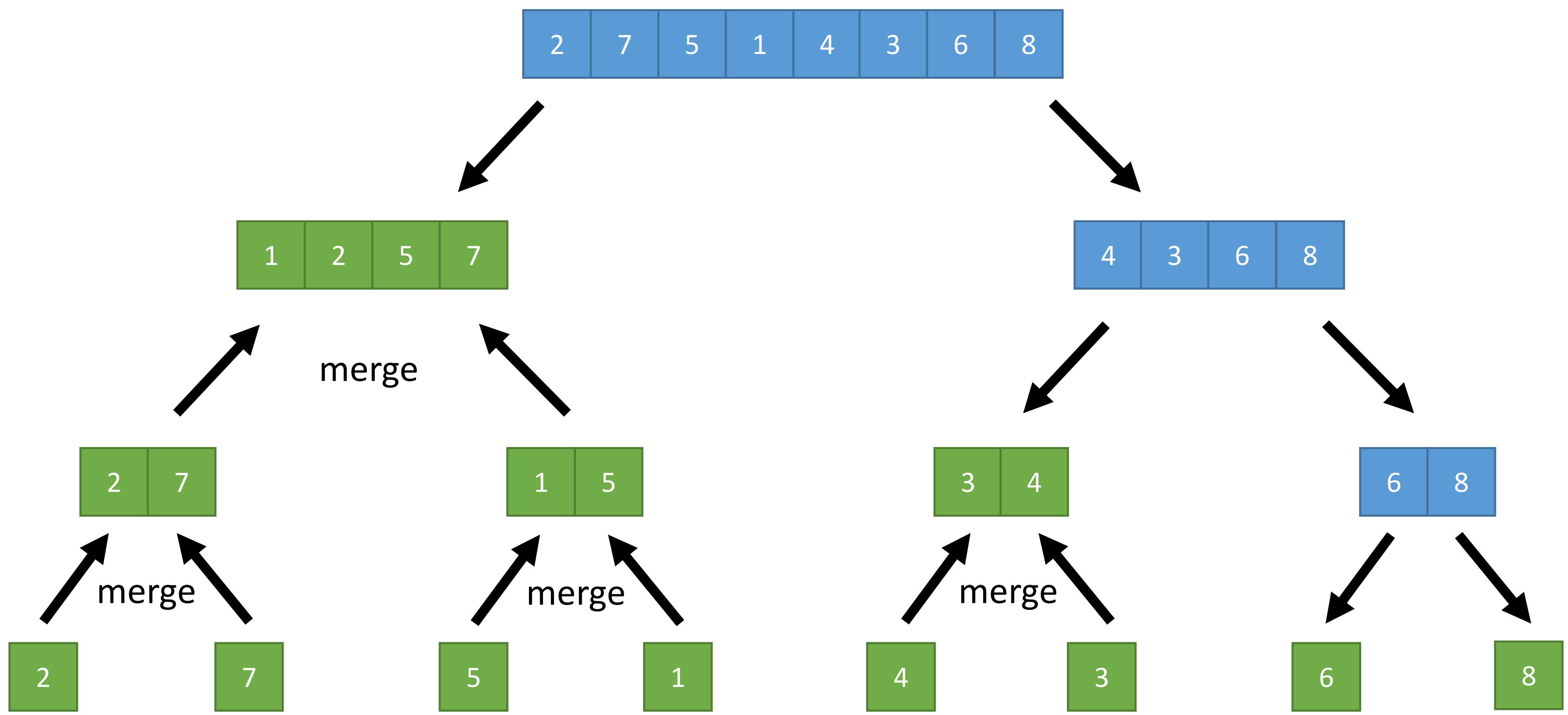
2 7 5 1 4 3 6 8
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merge
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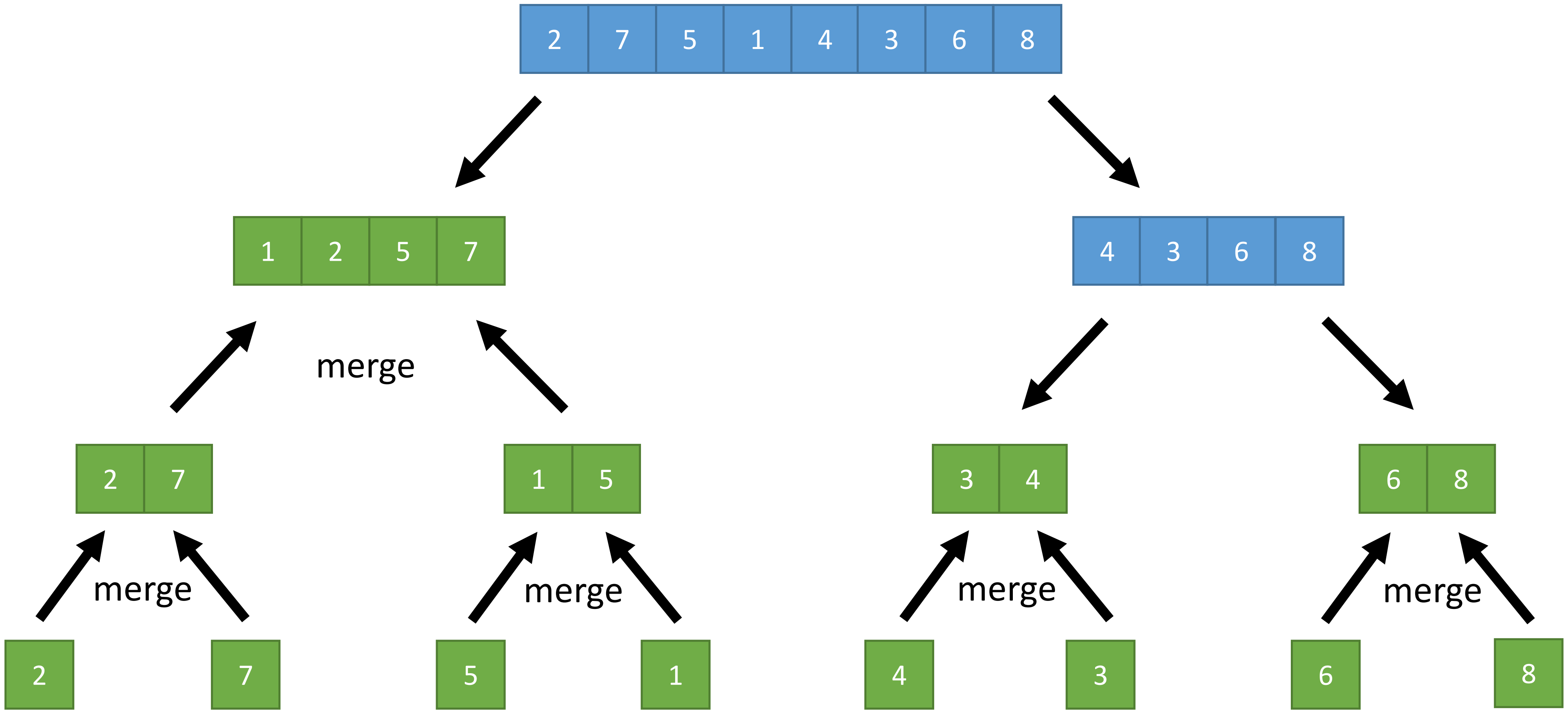
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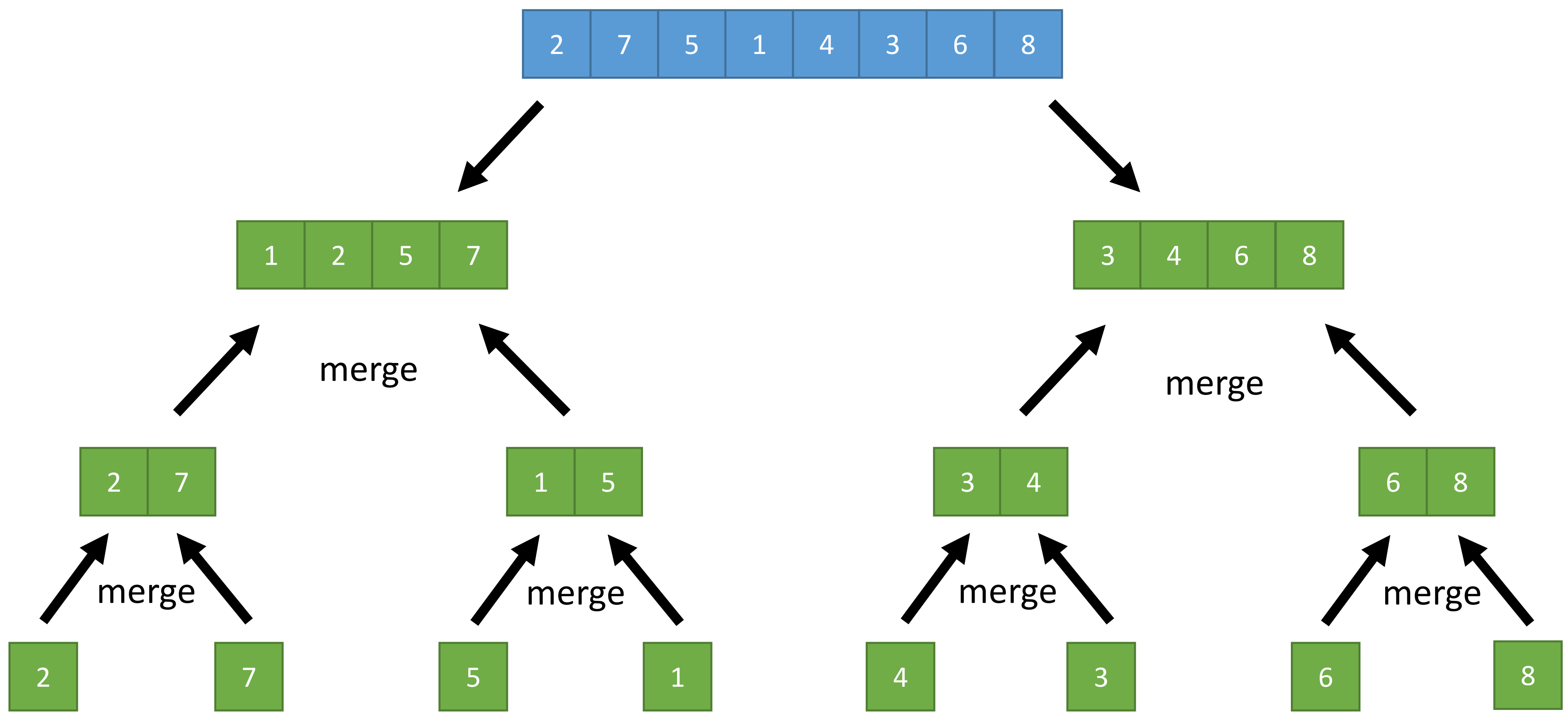

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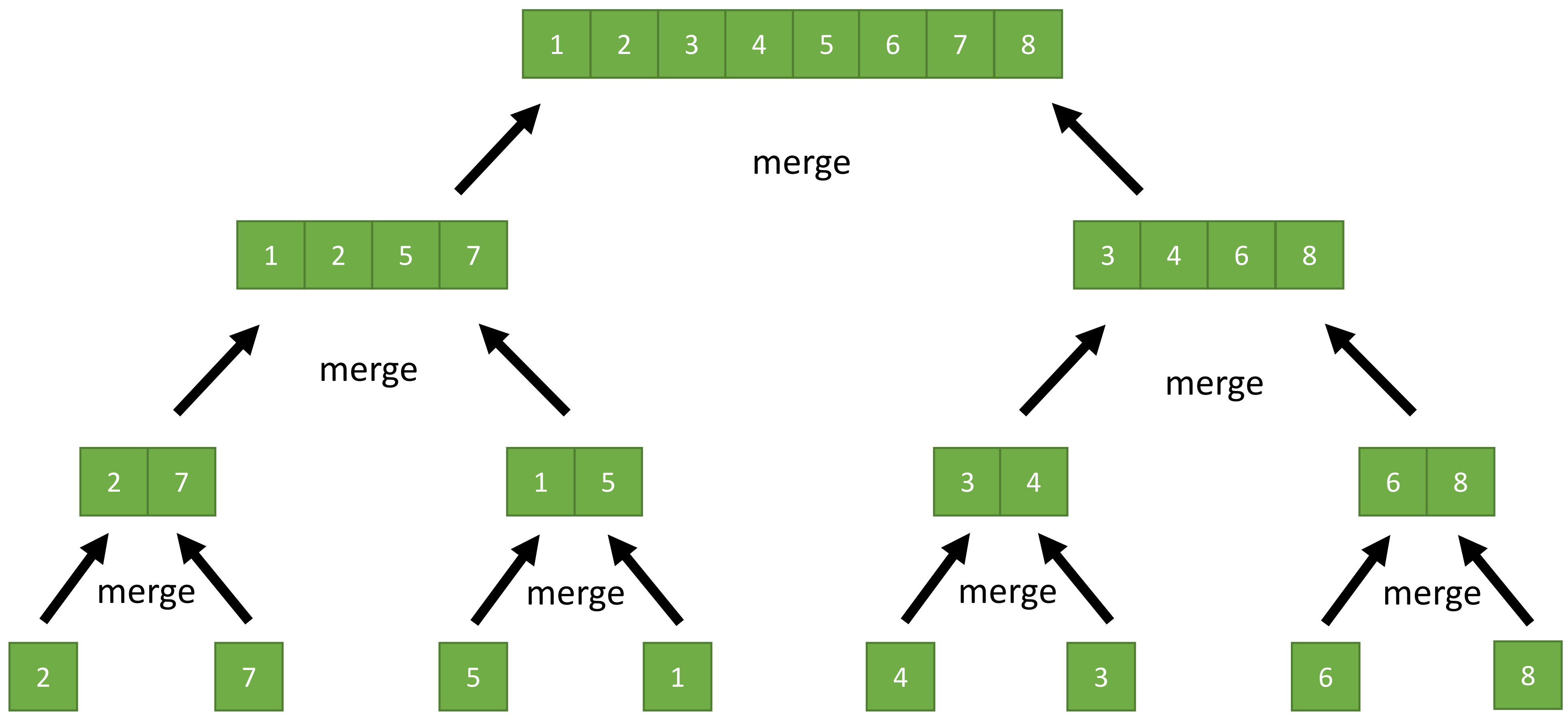
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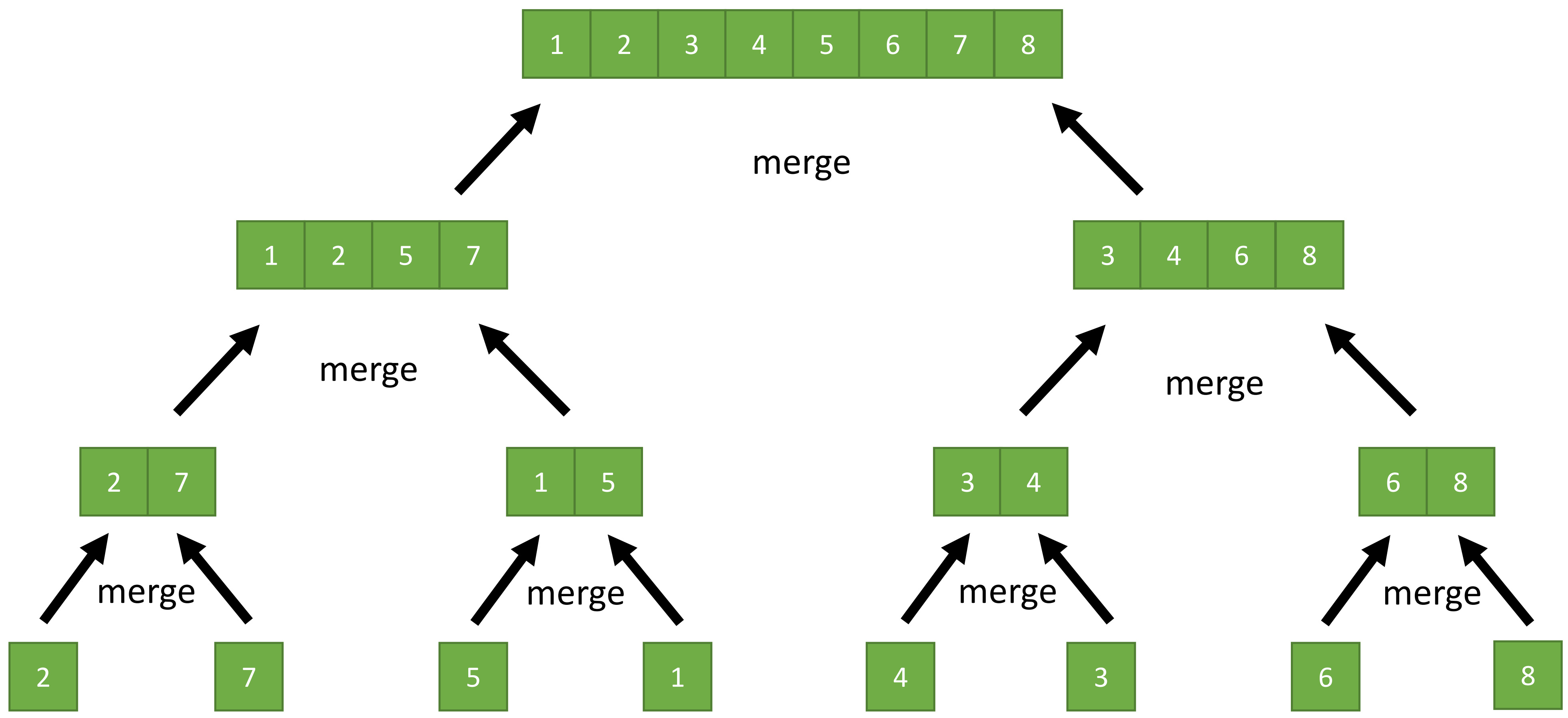
# Merge Sort

$O(N \log N)$



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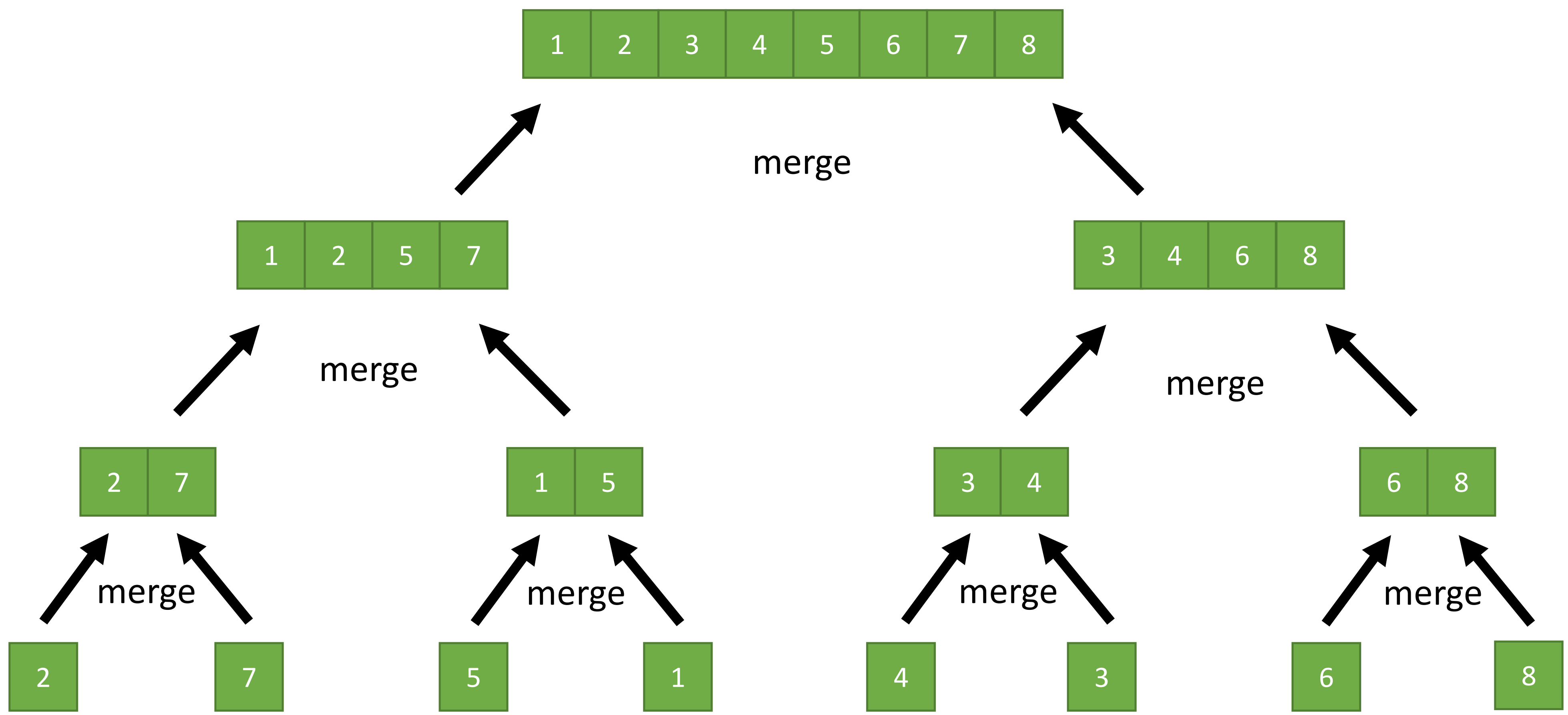



15 Sorting Algorithms in 6 Minutes

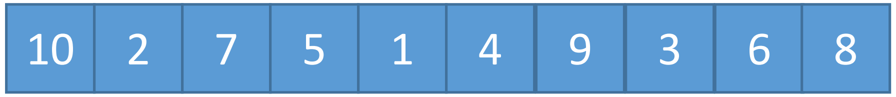
http://youtu.be/kPRA0W1kECg

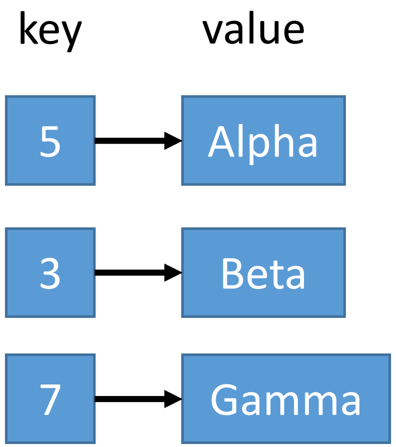
http://bigocheatsheet.com/

Nicolai Josuttis, The C++ Standard Library.

# Data structure complexity

# Data Structures




Sequence

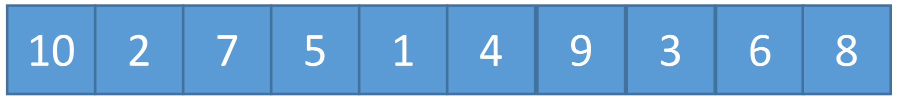
Associative

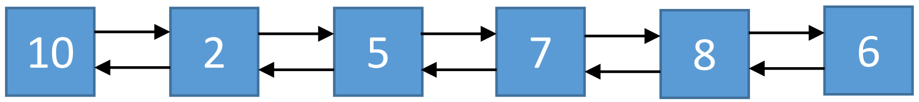
e.g., C-Arrays, std::vector, std::deque, std::list

e.g., C-Arrays, std::map, std::set, std::unordered_map

# Data Structures

- Operations:
  - Insertion
  - Searching
  - Deletion
- Variants:
  - Ordered
  - Unordered




# Sequential Containers

Arrays, Lists, Queues, Stacks

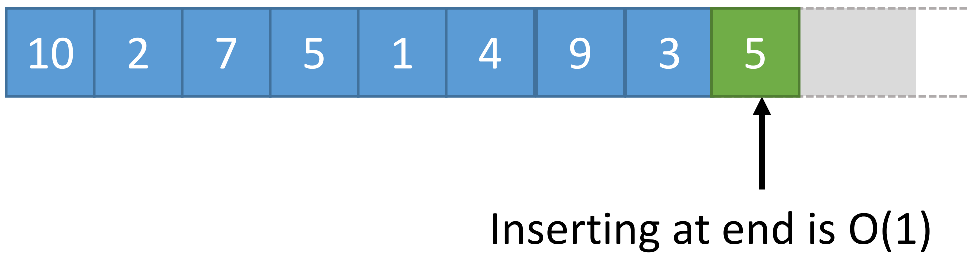
# STL Containers

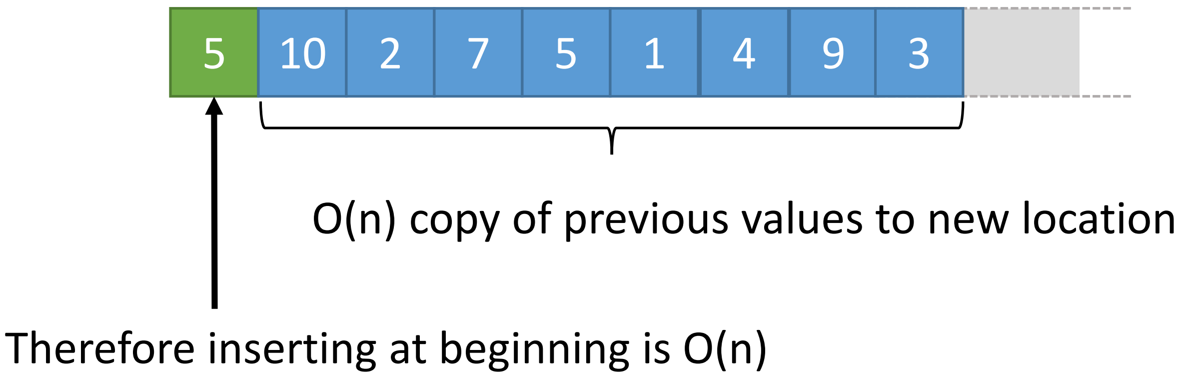
- Sequence Containers
  - vector (flexible sequence)
  - deque (double-ended queue)
  - list (double linked list)
  - array (fixed sequence, C++11)
  - forward_list (single linked list, C++11)

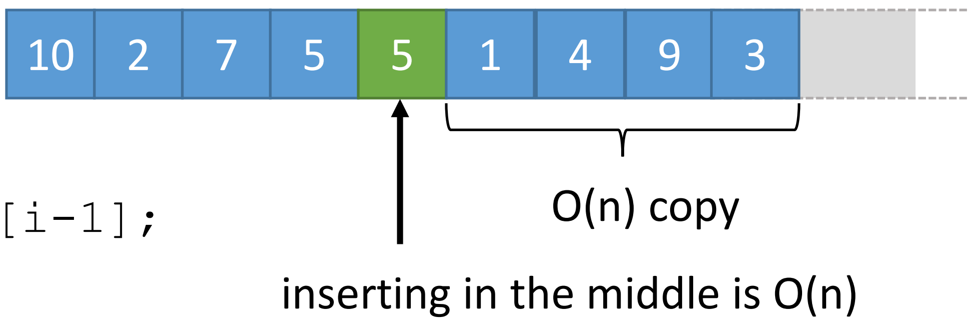
# C-Arrays

- Simplest Sequence Data Structure
- Data stored in range [0, numElements)
- Fixed Size, Wasteful
- Consecutive Memory (efficient access)

```
int a[10000];
int numElements = 0;

// insertion at end O(1)
a[numElements++] = new_value;

// insertion at beginning O(n)
for(int i = numElements; i > 0; i--) a[i] = a[i-1];
a[0] = new_value;
numElements++;
```



# std::vector

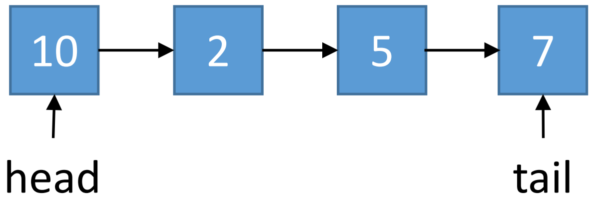
```
#include <iostream>
#include <vector>

using namespace std;

// empty construction
vector<int> a;
// sized construction
vector<int> a(10);
// sized construction with initial value
vector<int> a(100, -1);
// C++ 11 initializer lists
vector<int> a { 3, 5, 7, 9, 11 };

// insertion at end
a.push_back(3);
a.push_back(5);
a.push_back(7);

// delete at end
a.pop_back();

// insertion at beginning
a.insert(a.begin(), new_value);
```

```
// accessing elements just like arrays
for(int i = 0; i < a.size(); i++) {
   cout << a[i] << endl;
}

// using iterators
for(auto i = a.begin(); i != a.end(); ++i) {
   cout << *i << endl;
}

// C++11 for each
for(auto element : a) {
   cout << element << endl;
}
```

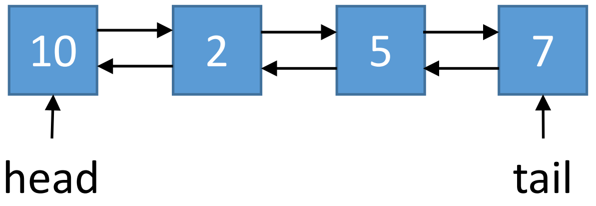
# Linked-List

- List Elements connected through pointers
- First Element (head) and last element (tail) are always known
- Insertion/Deletion at **both** ends in O(1)
- Insertion in the middle is also cheaper
  - Finding insertion location is O(n) compared to O(1) with C-Arrays
  - But insertion itself happens in O(n) instead of O(n) copies
- Dynamic Size
- Distributed in memory

**Single Linked-List**:
only pointer of next element




**Double Linked-List**:
pointer of previous and next element




```
struct Node {
    Node * prev;
    Node * next;
    int data;
}
```

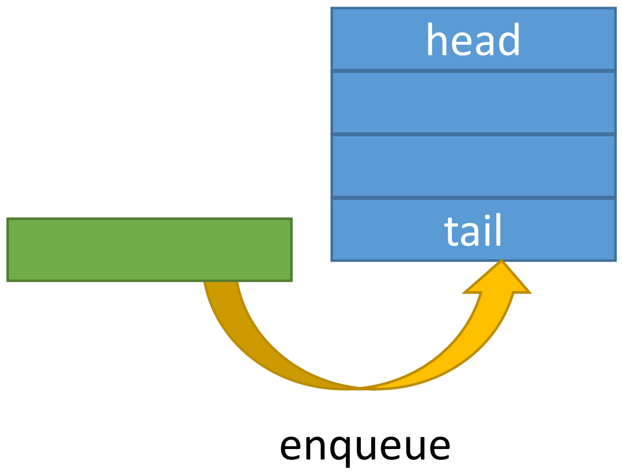
# std::list

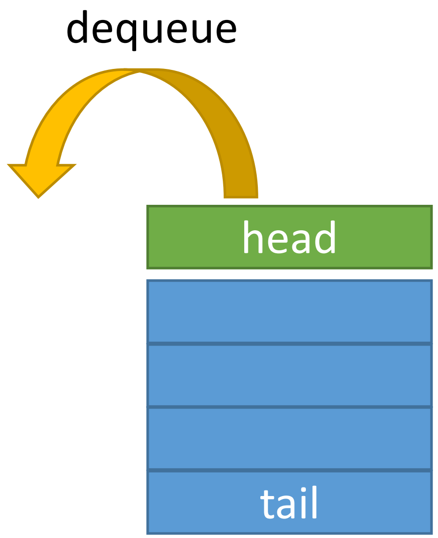
```
#include <iostream>
#include <list>

using namespace std;

// empty construction
list<int> a;
// sized construction
list<int> a(10);
// sized construction with initial value
list<int> a(100, -1);
// C++ 11 initializer lists
list<int> a { 3, 5, 7, 9, 11 };

// insertion at beginning
a.push_front(3);

// insertion at end
a.push_back(3);

// delete at beginning
a.pop_front();

// delete at end
a.pop_back();
```

```
// access front element
int first = a.front();

// access last element
int last = a.back();

// using iterators
for(auto i = a.begin(); i != a.end(); ++i) {
   cout << *i << endl;
}

// C++11 for each
for(auto element : a) {
   cout << element << endl;
}
```

# Queue

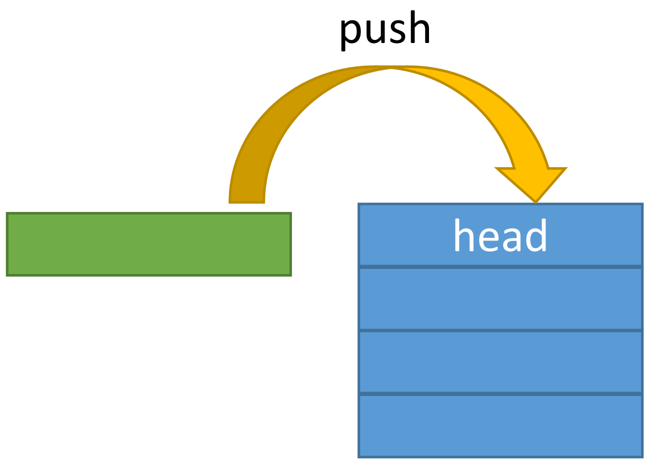
- First-In-First-Out (FIFO) data structure
- Implementations:
  - Double-Linked-List
- Operations:
  - **enqueue**: put element in queue (insert at tail)
  - **dequeue**: get first element in queue (remove head)

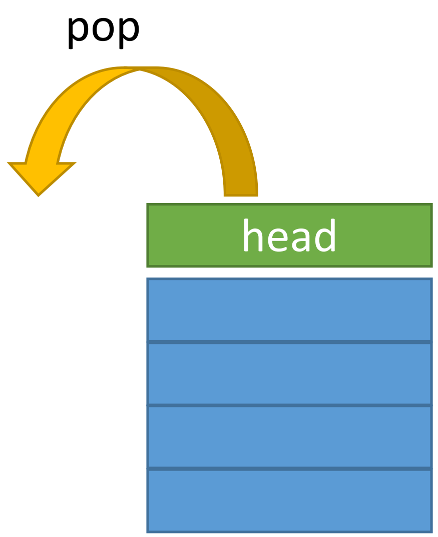


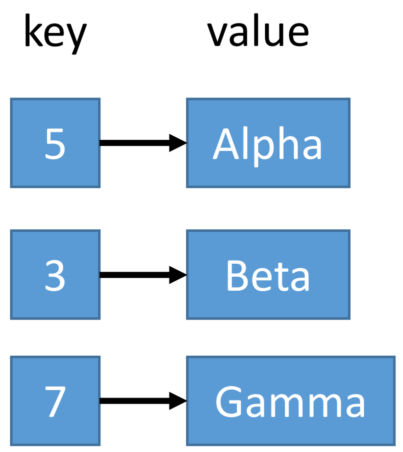



# Stack

- Last-In-First-Out (LIFO) data structure
- Implementations:
  - C-Array
  - Single-Linked-List
- Operations:
  - **push**: put element on stack (insert as first element)
  - **pop**: get first element on stack (remove head)






# Associative Containers

Dictionaries, Maps, Sets

# Associative Containers

- Map a key to a value
- Searching for a specific element in unsorted sequential containers takes **linear** time O(n)
- Getting a specific element from an associative container can be as fast as **constant** time O(1)

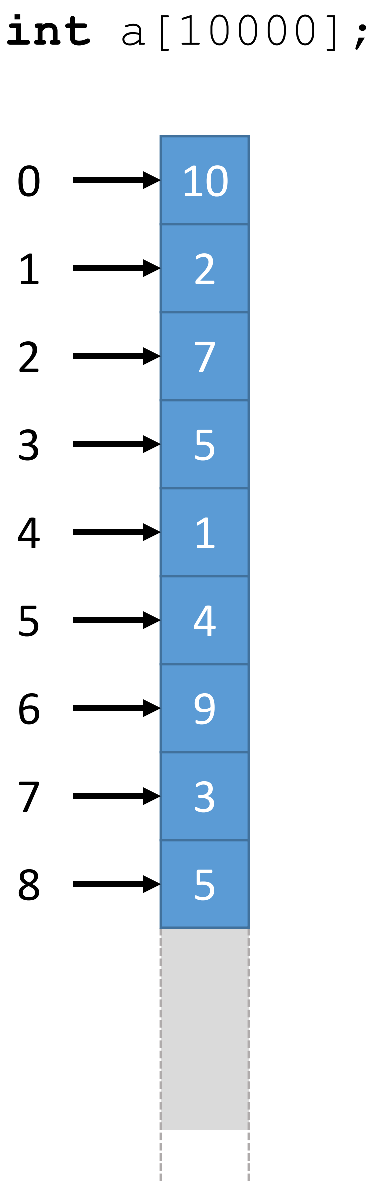
# STL Containers

- Associative Containers
    - map
    - set
    - multimap
    - multiset

    - unordered_map (C++11)
    - unordered_set (C++11)
    - unordered_multimap (C++11)
    - unordered_multiset (C++11)

# C-Array as Associative Container

- Simplest associative data structure
- maps **integer number** to data
  - 0 -> a[0]
  - 1 -> a[1]
  - …
- **efficient access in O(1)**
- **inefficient storage**
- **limited to positive integer numbers as keys**



# Ordered maps

- Maps **arbitrary keys** (objects, basic types) to **arbitrary values** (objects, basic types)
- Basic idea: if keys are sortable, we can store nodes in a data structure sorted by its keys. Sorted data structures can be searched more quickly, e.g. with binary search in O(log(n))
- Elements ordered by key
- **Worst case lookup time is O(log(n))**

# std::map

```
#include <iostream>
#include <map>
#include <string>

using namespace std;

map<string, string> capitals;

// setting value for key
capitals["Austria"] = "Vienna";
capitals["France"] = "Paris";
capitals["Italy"] = "Rome";

// getting value from key
cout << "Capital of Austria: " << capitals["Austria"] << endl;
string & capital_of_france = capitals["France"];
cout << "Capital of France: " << capitals << endl;


// check if key is set
if (capitals.find("Spain") != capitals.end()) {
    cout << "Capital of Spain is " << capitals["Spain"]  << endl;
else {
    cout << "Capital of Spain not found!" << endl;
}
```

# std::map

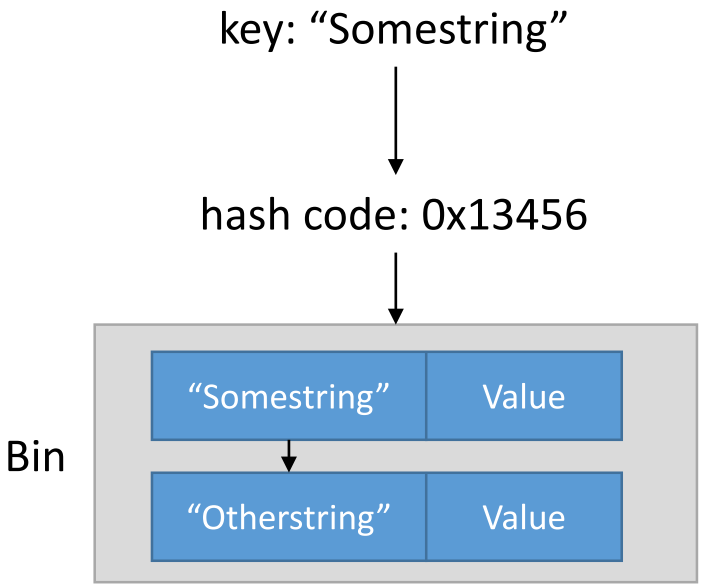
```
// iterate over all elements
for (map<string, string>::iterator it = capitals.begin(); it != capitals.end(); ++it) {
    string & key = it->first;
    string & value = it->second;
    cout << "The capitol of " << key << " is " << value << endl;
}

// C++11: iterate over all elements
for (auto it = capitals.begin(); it != capitals.end(); ++it) {
    string & key = it->first;
    string & value = it->second;
    cout << "The capitol of " << key << " is " << value << endl;
}

// C++11: iterate over all elements
for (auto & kv : capitals) {
    string & key = kv.first;
    string & value = kv.second;
    cout << "The capitol of " << key << " is " << value << endl;
}
```

# Unordered maps / Hash maps

**On average lookup times are O(1). But this is only true if there are only few hash collisions.**

Hash maps require **a good hashing function**, which reduces the amount of hash collisions.

- Maps **arbitrary keys** (objects, basic types) to **arbitrary values** (objects, basic types)
- **On average accessing a hash map through keys takes O(1)**
- In general unordered structure - you can't get out objects in the same order you inserted them.
- a number, called a **hash code**, is generated using a **hash function** based on key in O(1)
- Each hash code can be mapped to a location called a bin
- A bin stores nodes with keys which map to the same hash code
- Lookup therefore consists of:
  - Determining the hash code of the key  O(1)
  - Selecting the correct node inside the bin is in the worst case O(n)



# Reusability is an efficiency!

If the student after you has to start from 0,
nothing gained