High-level Optimization

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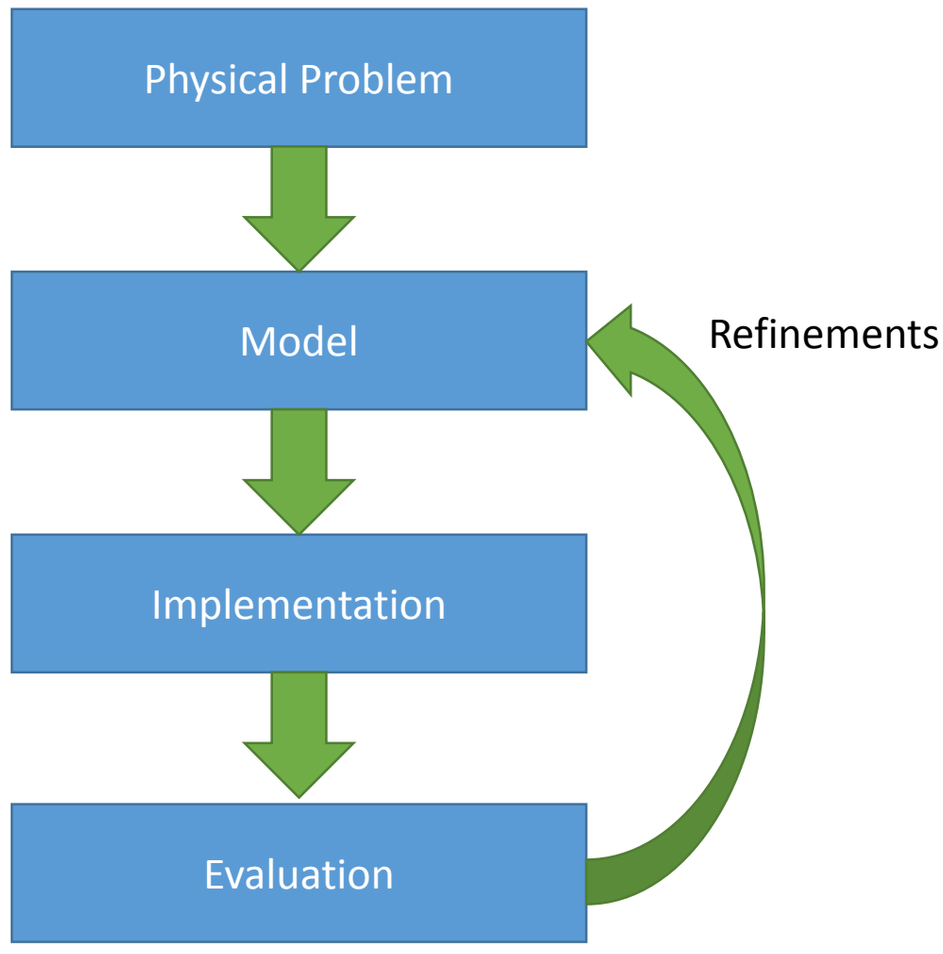
Typical scientific workflow

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)



Typical scientific workflow

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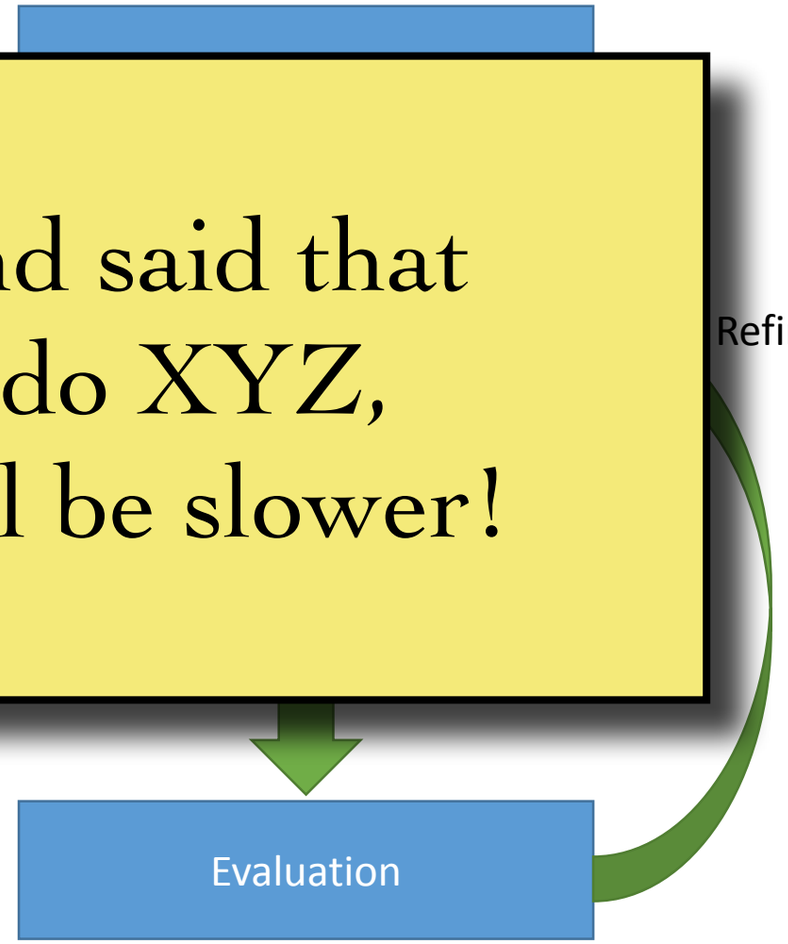
like it works is kept

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

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



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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!

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Reusability is an efficiency!

If the student after you has to start from zero,
all your work is wasted

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

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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, Prolog
to get an idea how different the approaches can be

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

now 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

- next lecture -

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Complexity basics

Much simplified, skipping formal derivation

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```
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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

Complexity basics

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$O(N\,N!)$

Scaling behaviour with size N of problem set:

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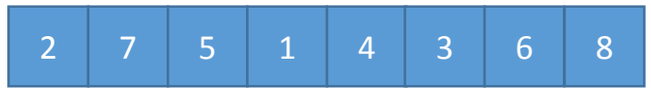
$O(N)$ - linear with N

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

Merge Sort



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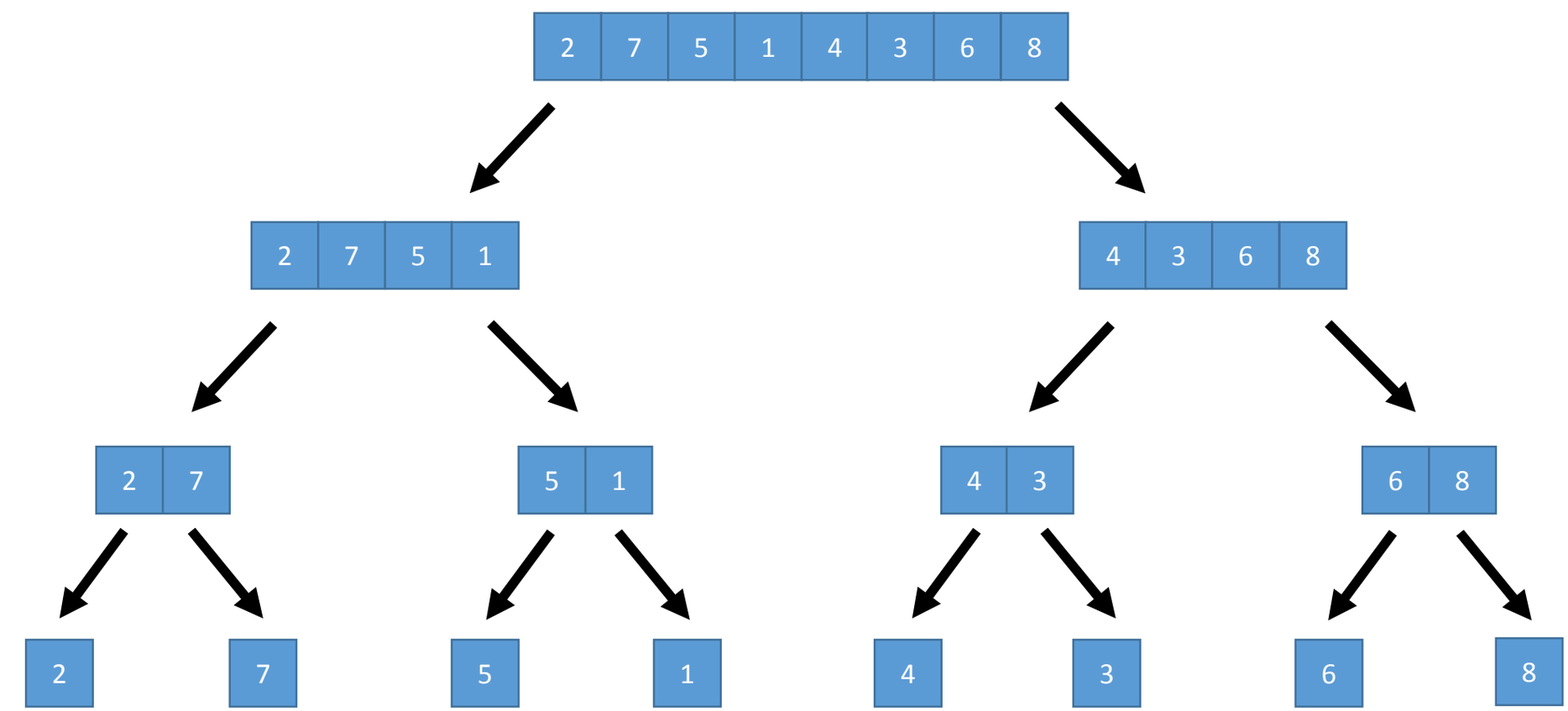

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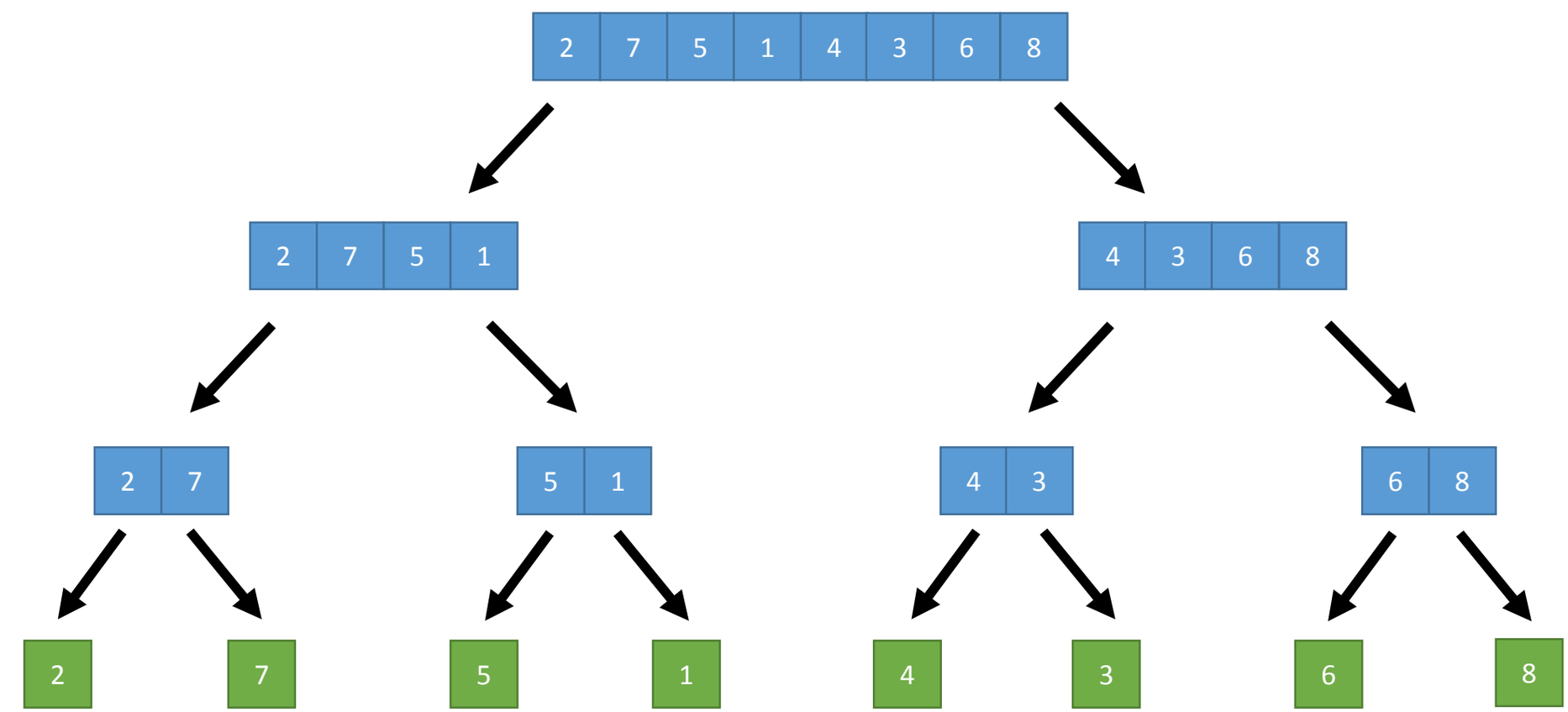

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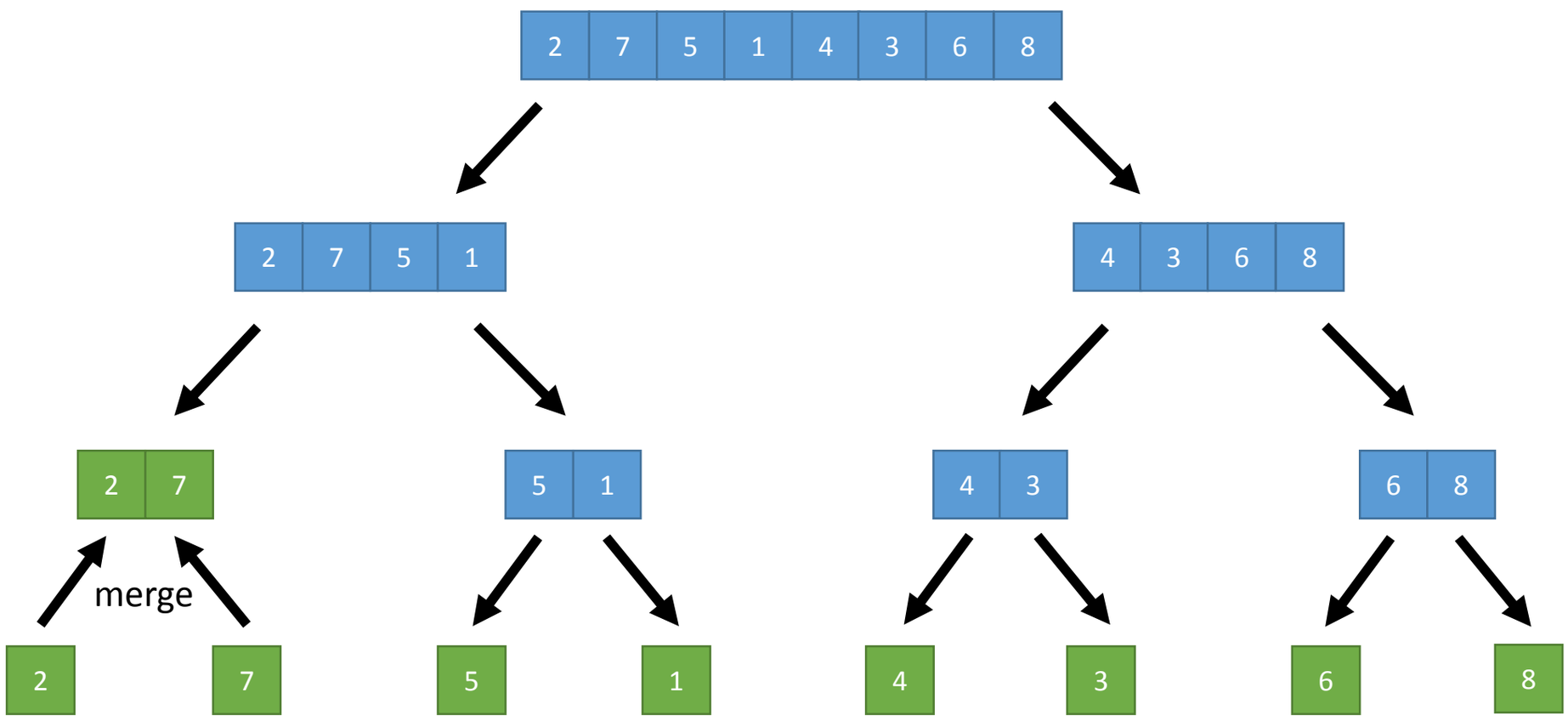

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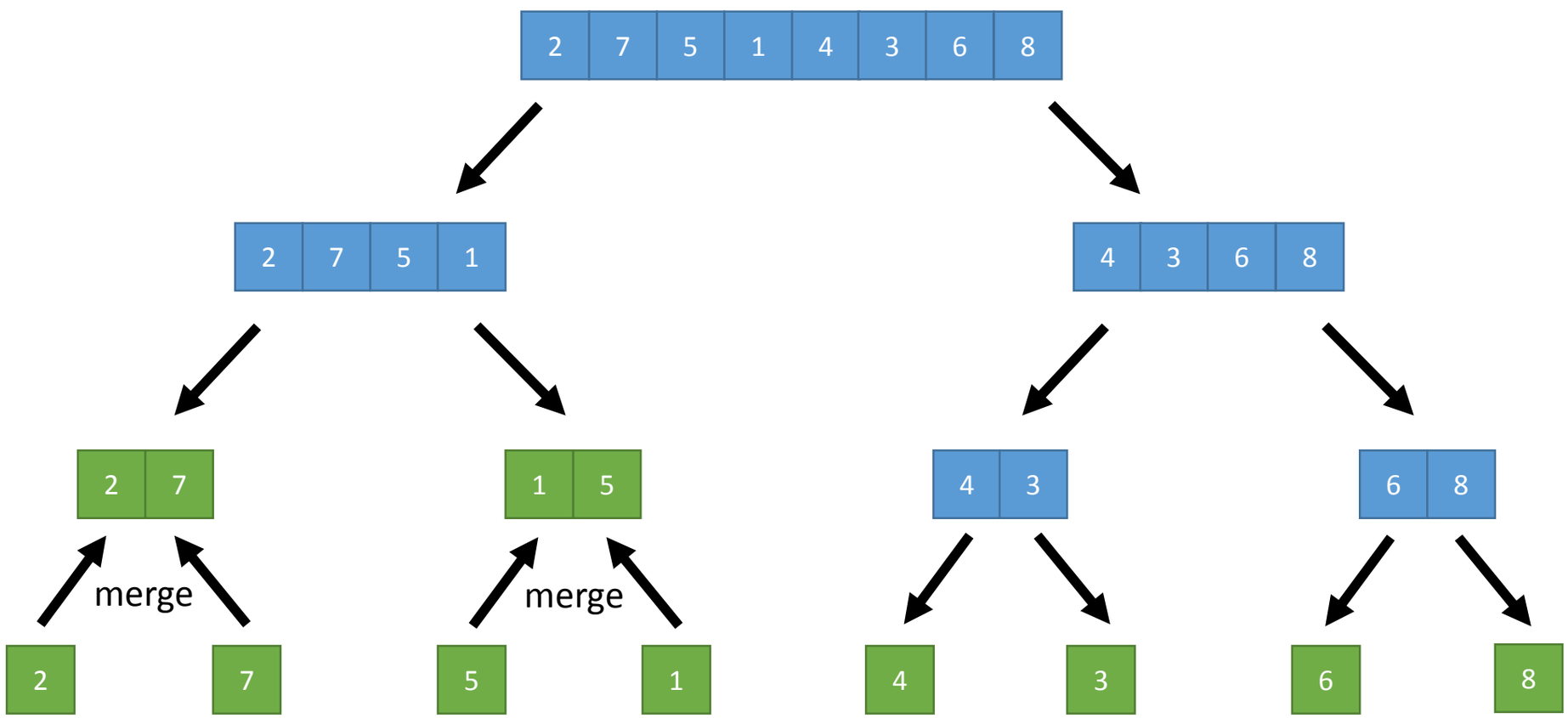

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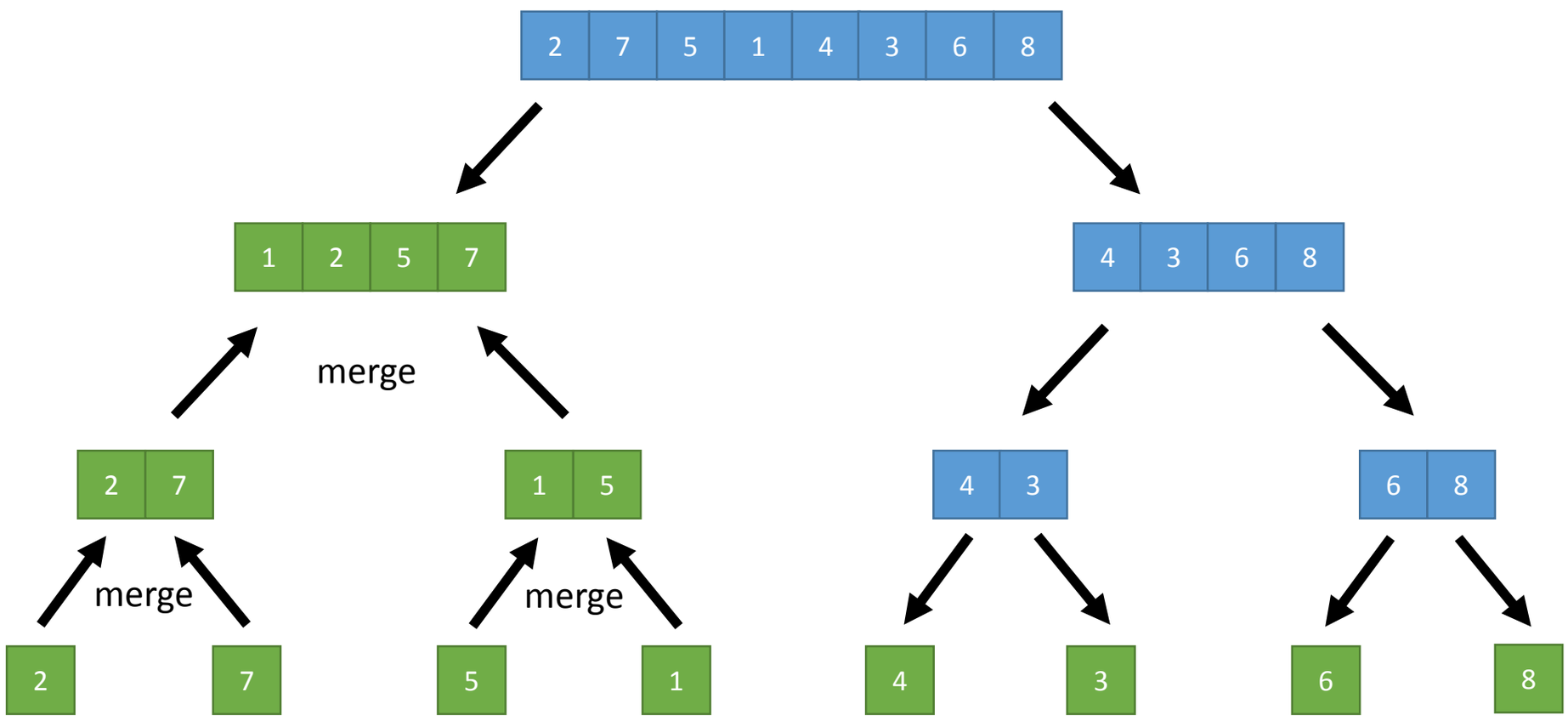

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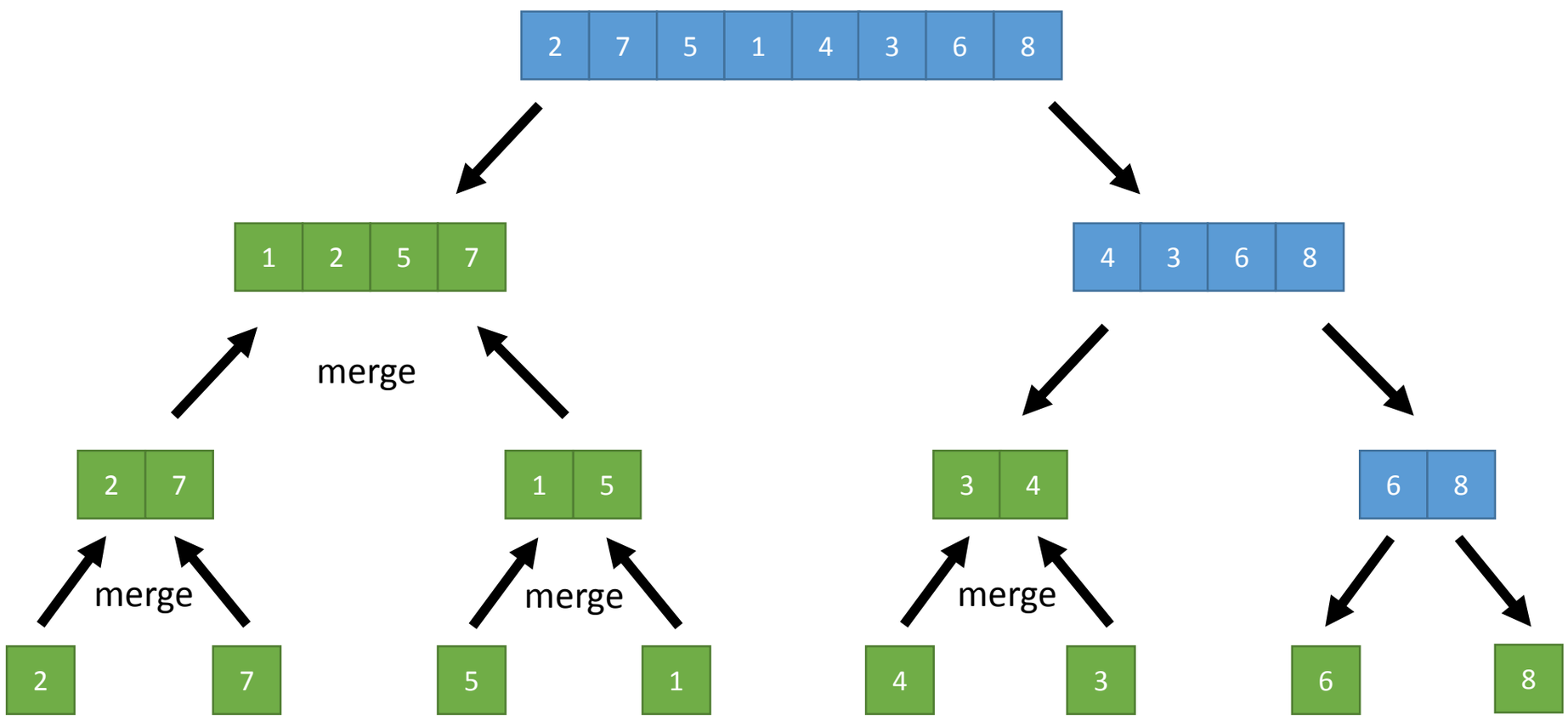
2 7 5 1 4 3 6 8
1 2 5 7
4 3 6 8
merge
2 7
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merge
merge
merge
2
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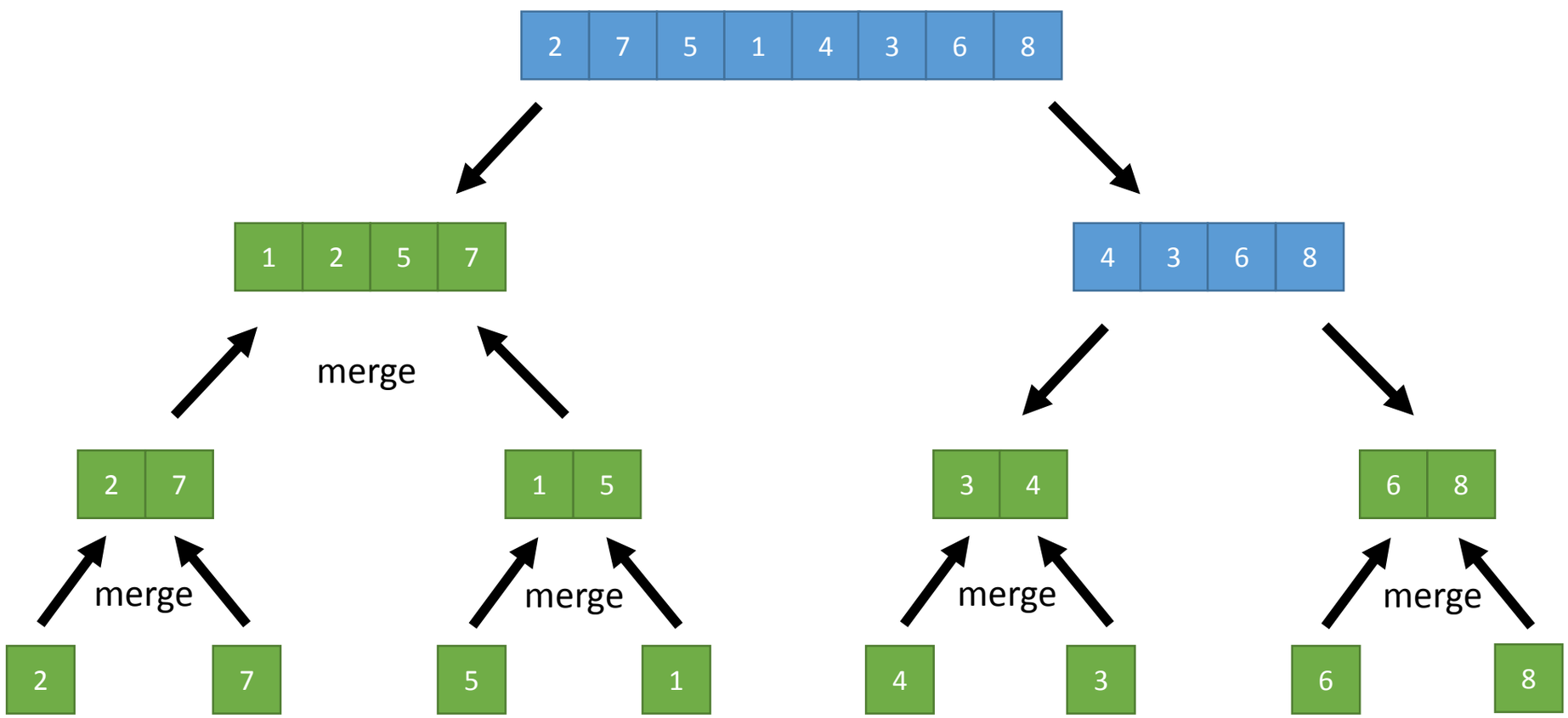
8

Merge Sort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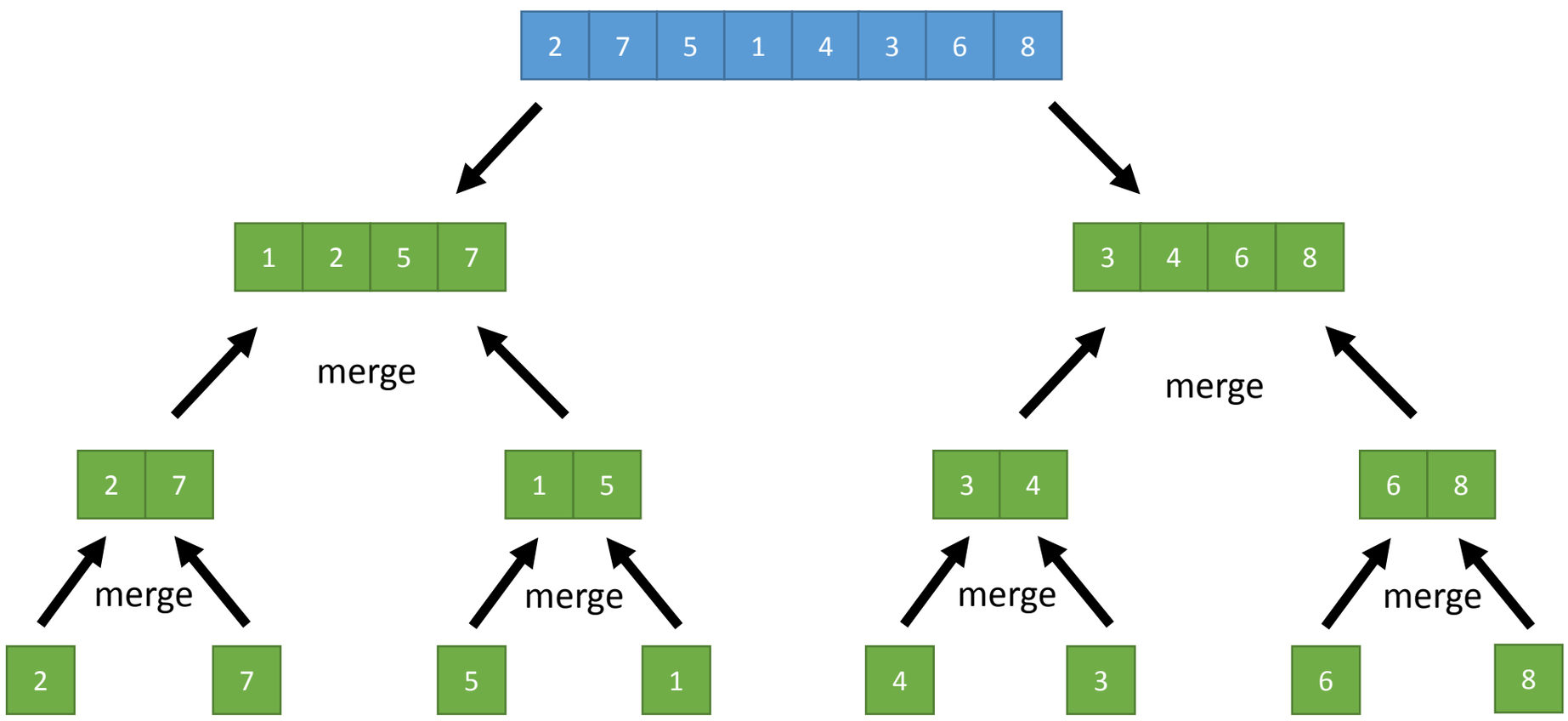
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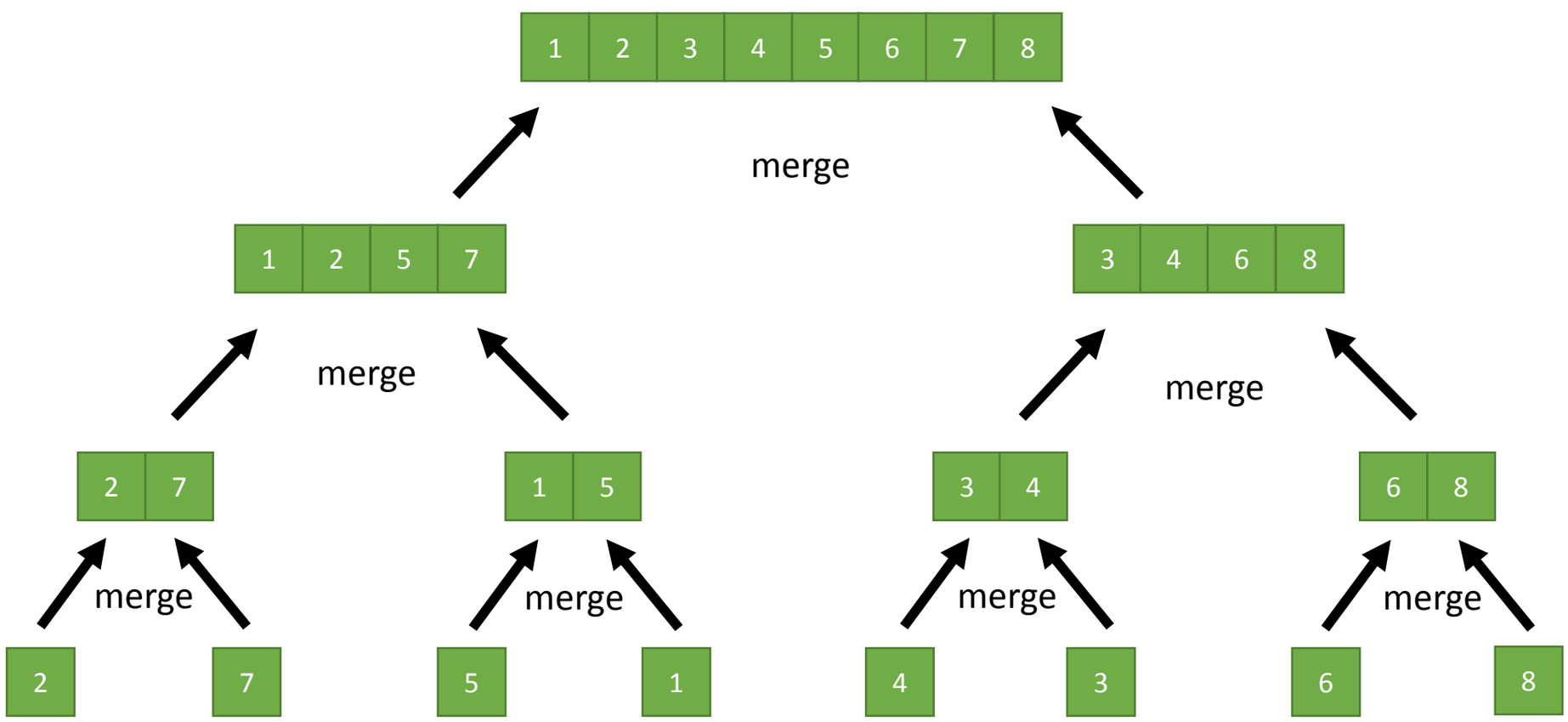
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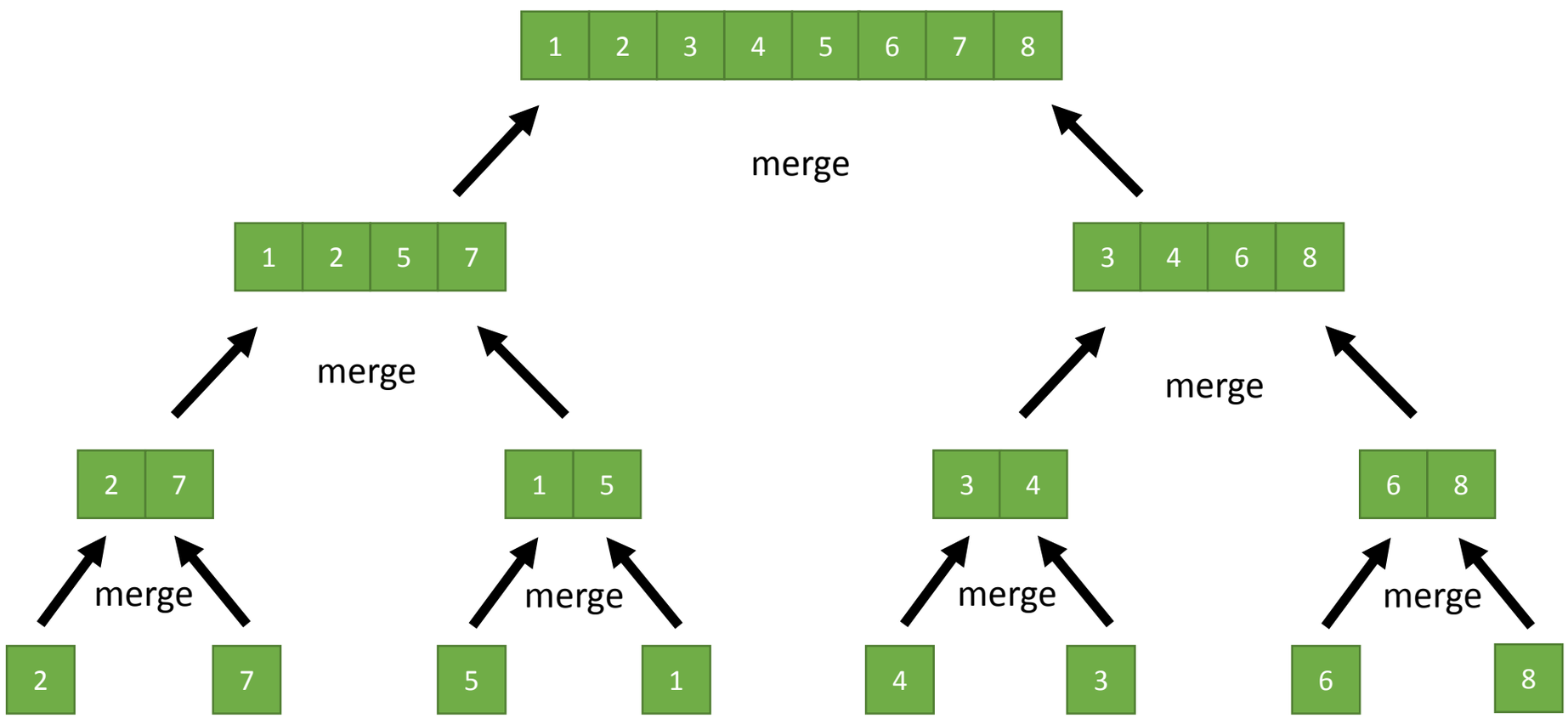
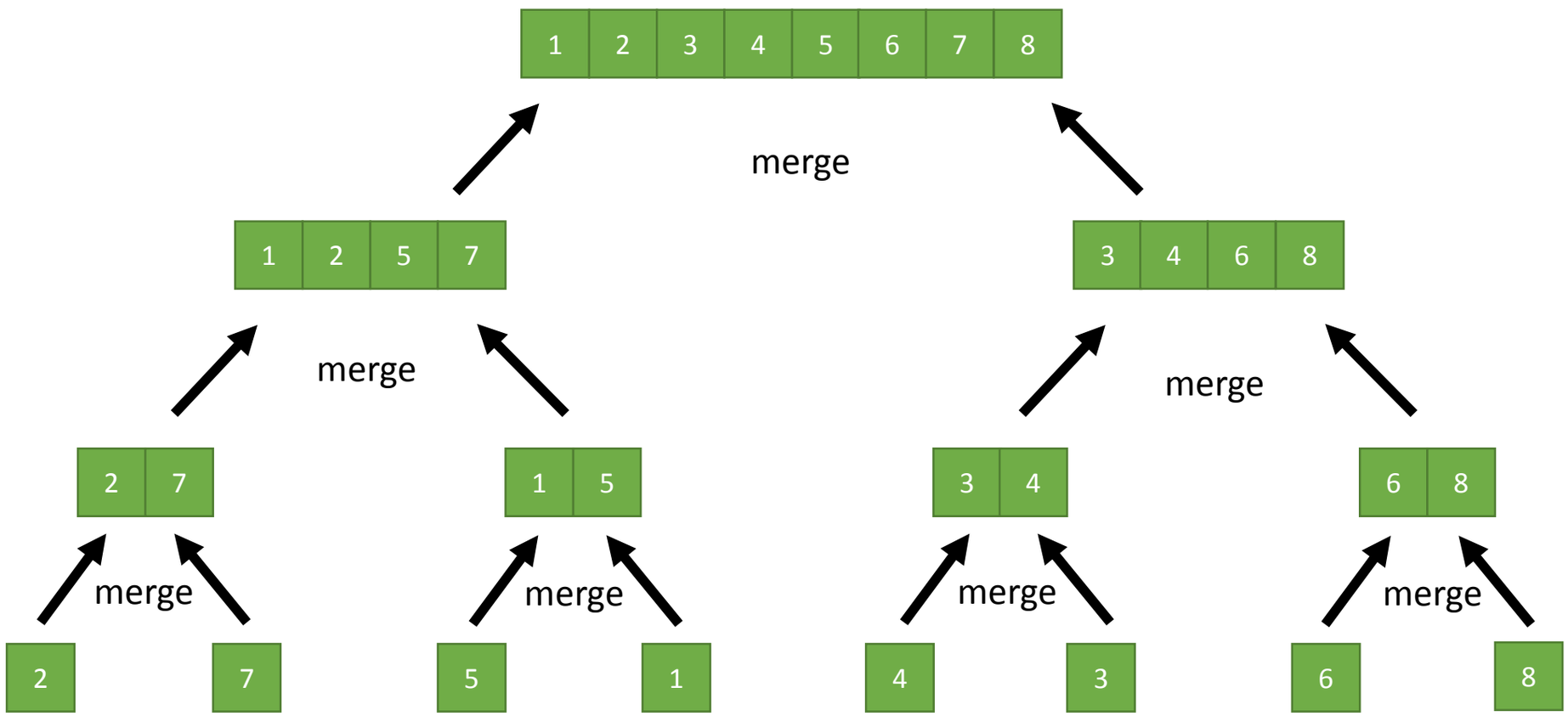
Merge Sort

$$\mathrm{O}(N \log N)$$



Merge Sort

$$O(N \log N)$$



15 Sorting Algorithms in 6 Minutes

http://youtu.be/kPRA0W1kECg

Data structure complexity

std::array
std::vector

std::list

std::map

std::unordered_map (hash table)

http://bigocheatsheet.com/
Nicolai Josuttis, “The C++ Standard Library”

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Numpy timing demo