High-level Optimization

David Grellscheid

Durham University

The Abdus Salam International Centre for Theoretical Physics

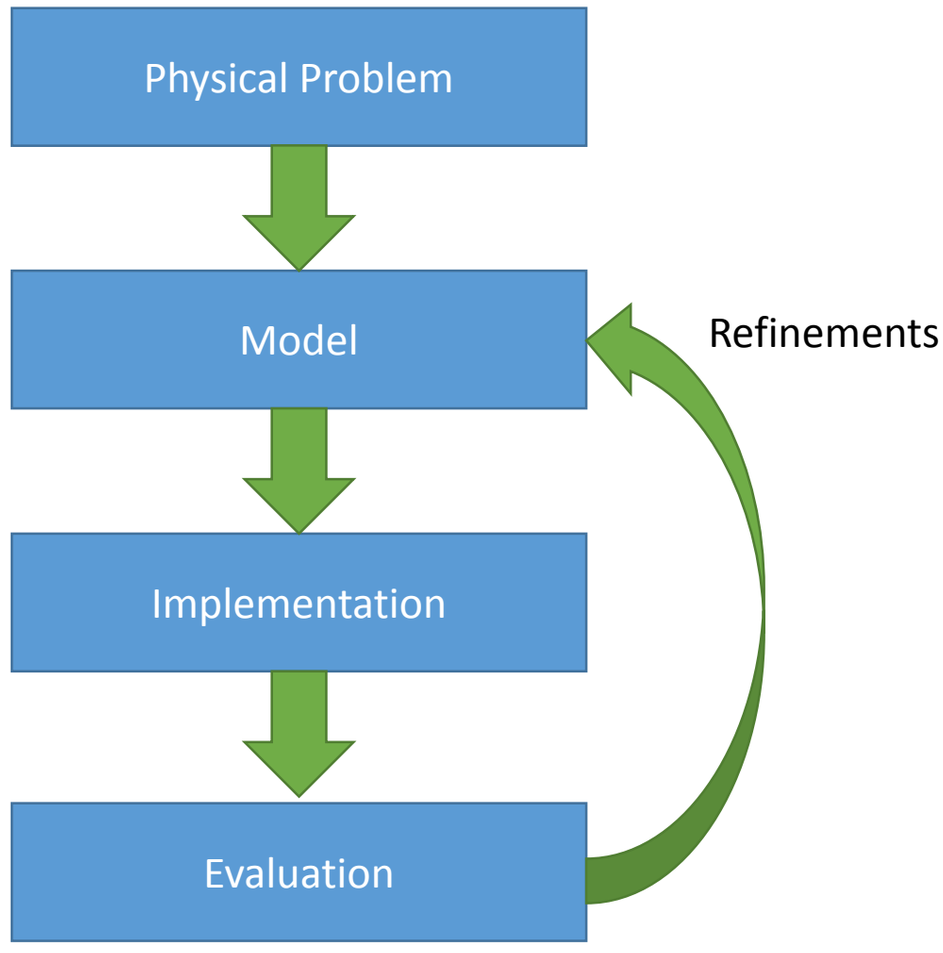
Typical scientific workflow

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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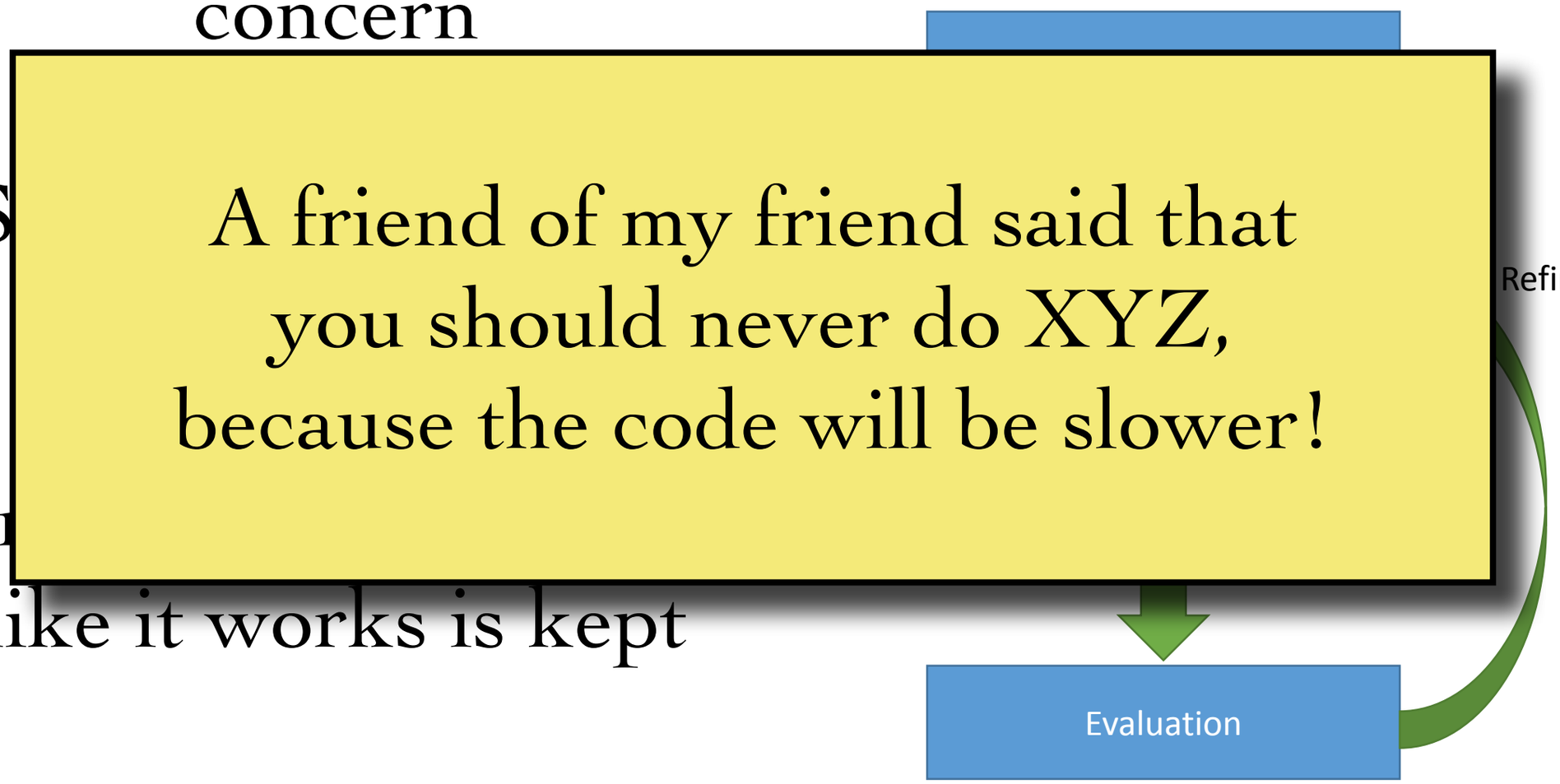

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Donald Knuth, December 1974:

> 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 0, nothing gained

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

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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

- next lecture -

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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

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$O(N\,N!)$

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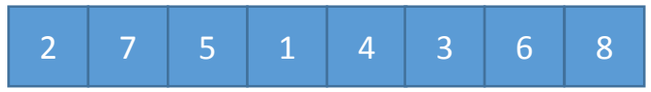
Merge Sort



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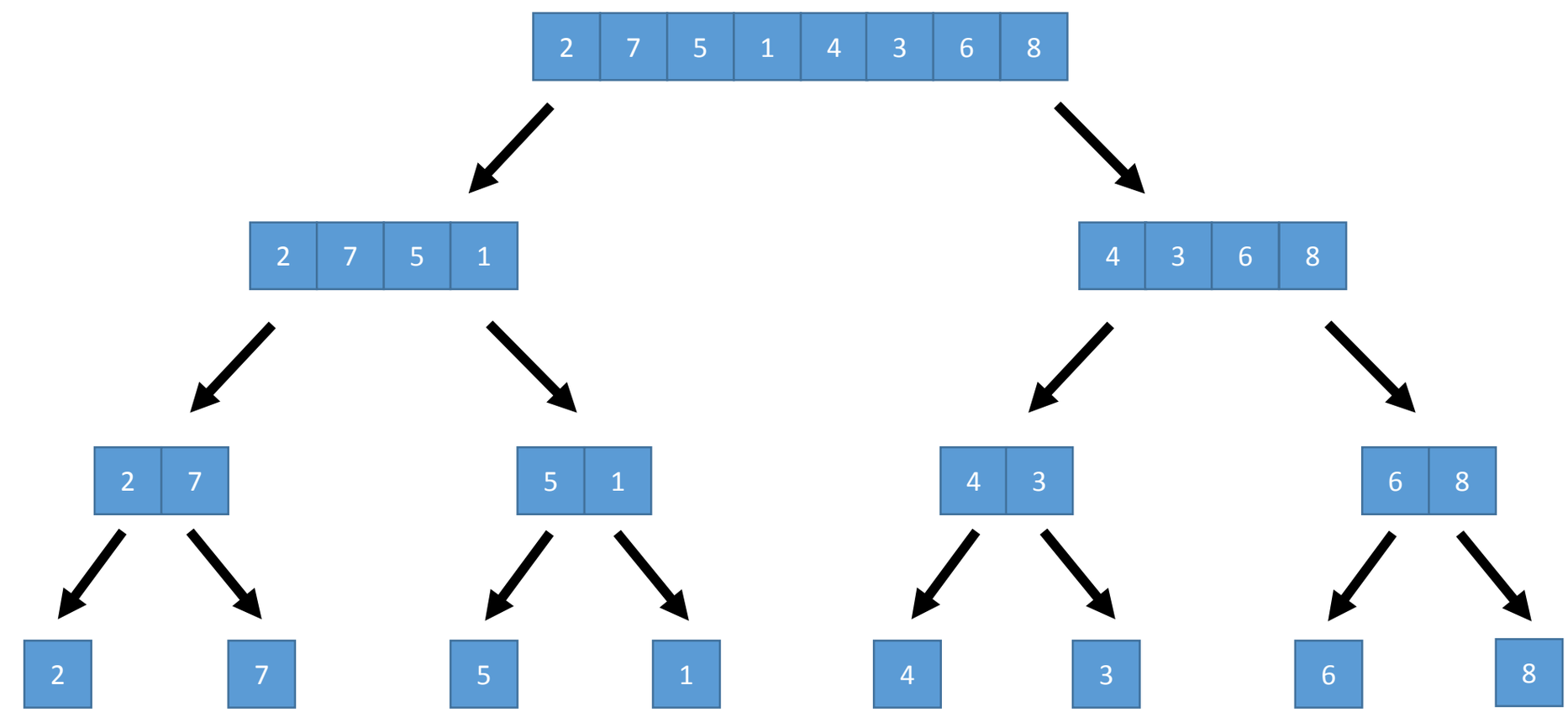

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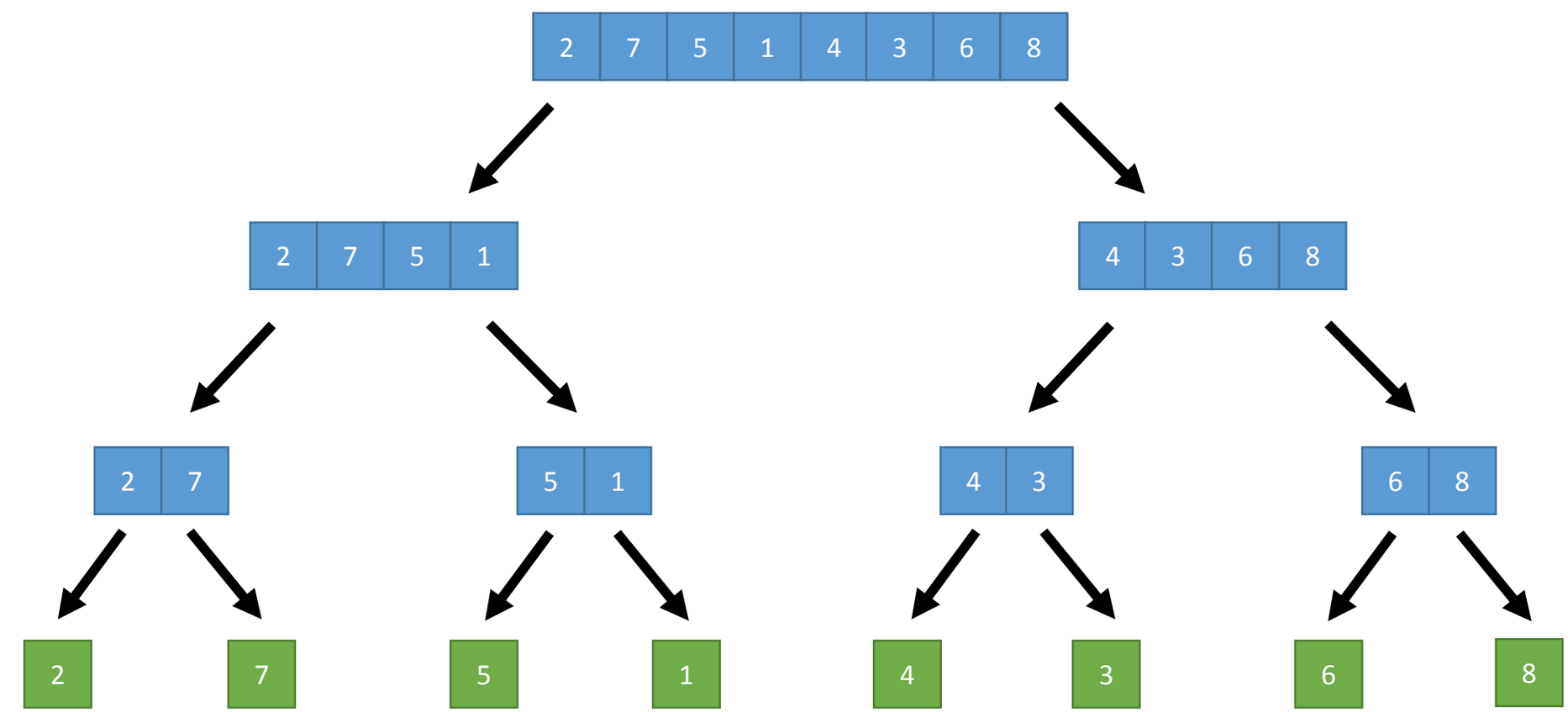

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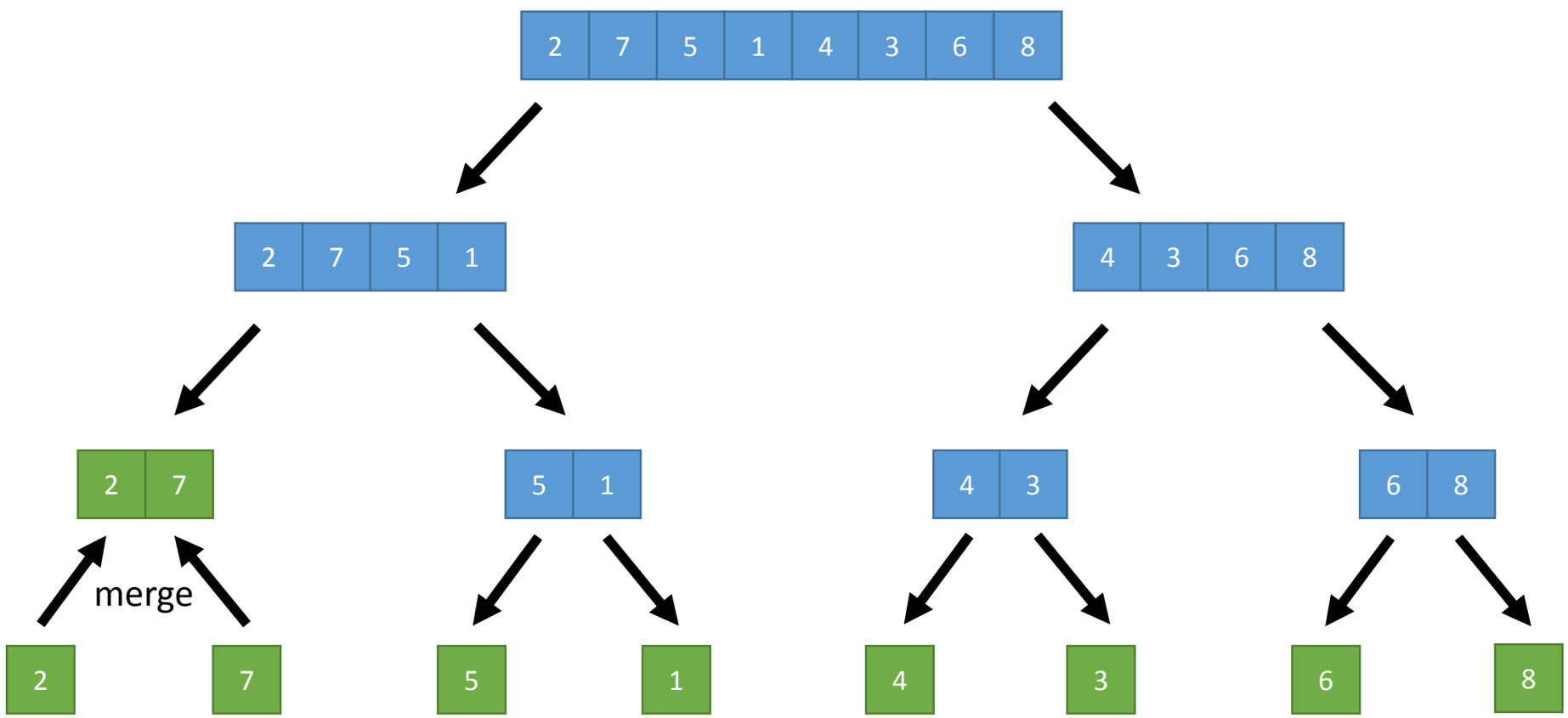

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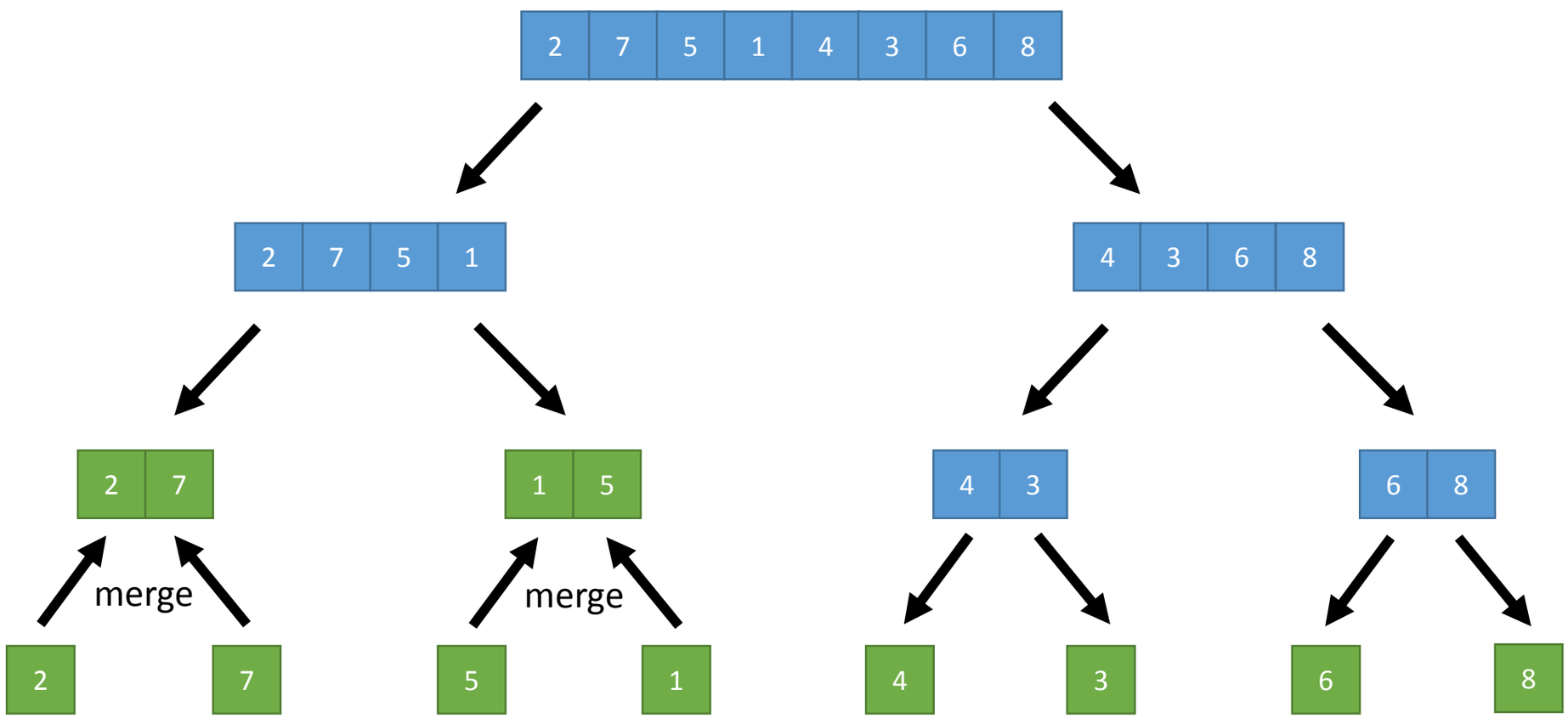

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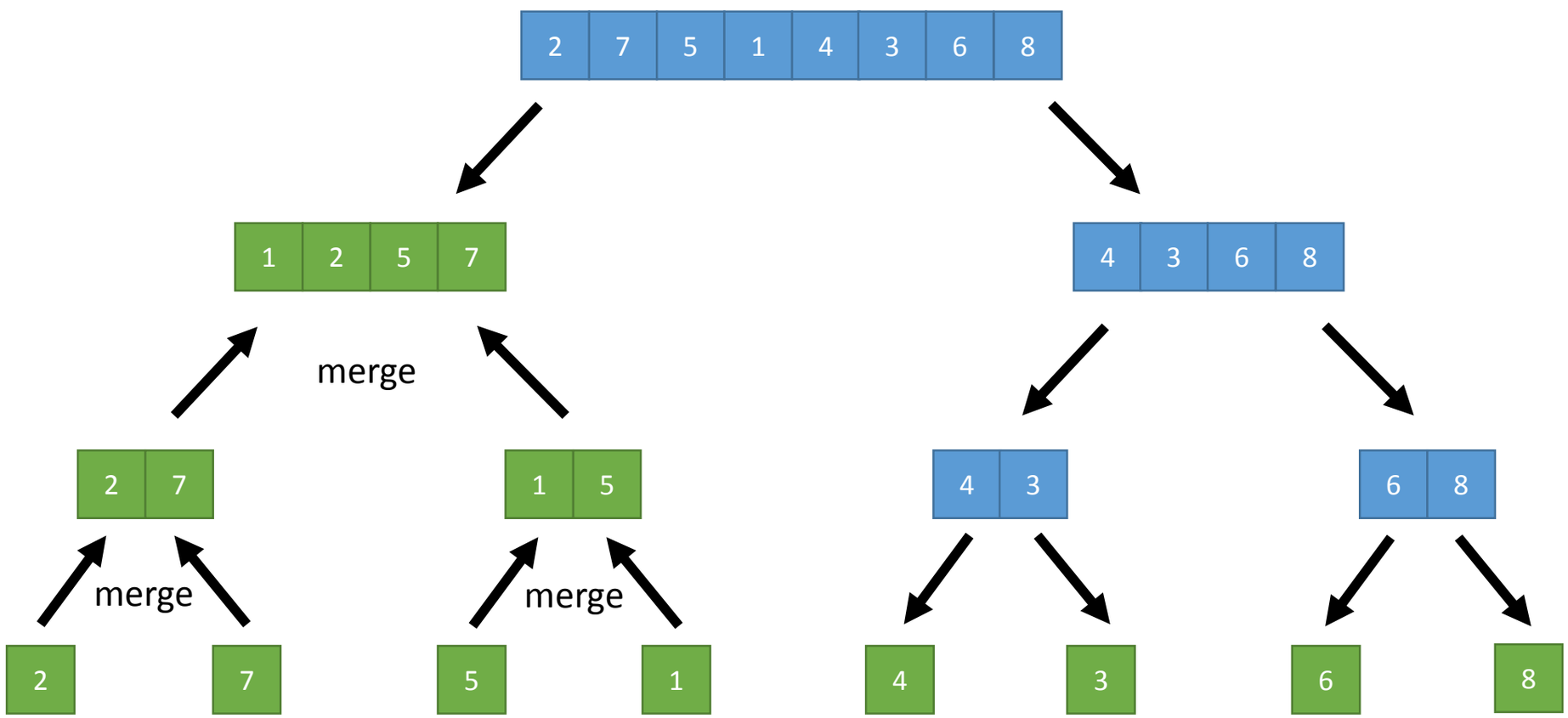

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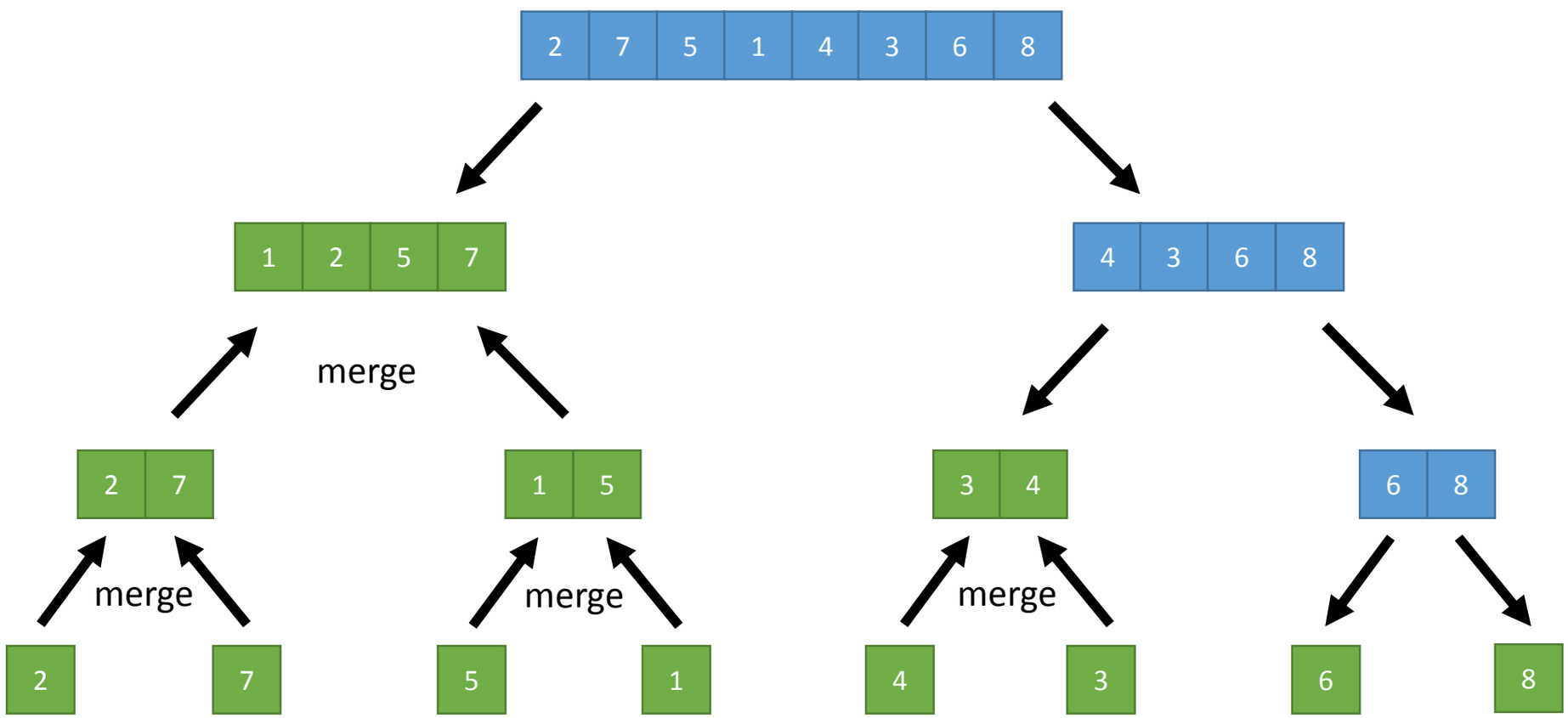
2 7 5 1 4 3 6 8
1 2 5 7
4 3 6 8
merge
2 7
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merge
merge
merge
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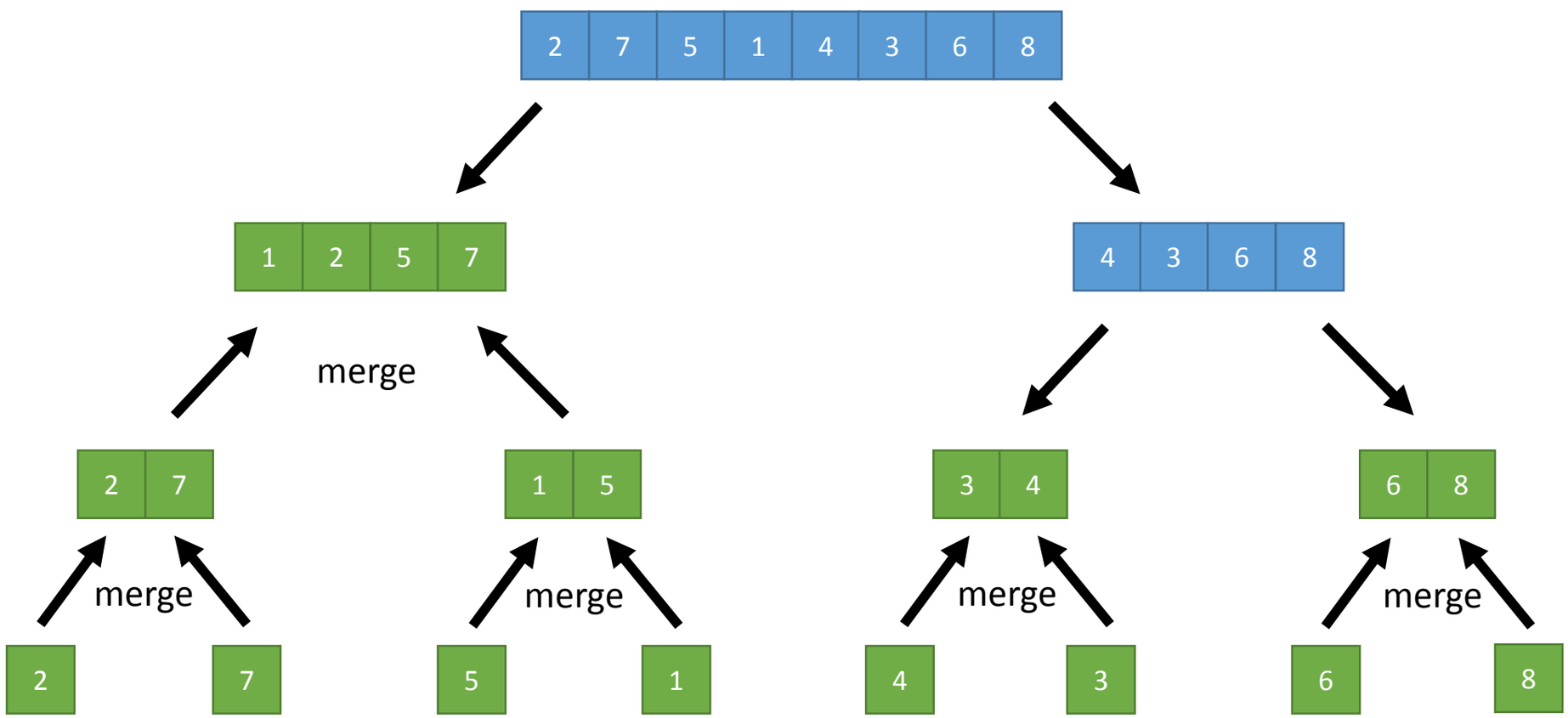
Merge Sort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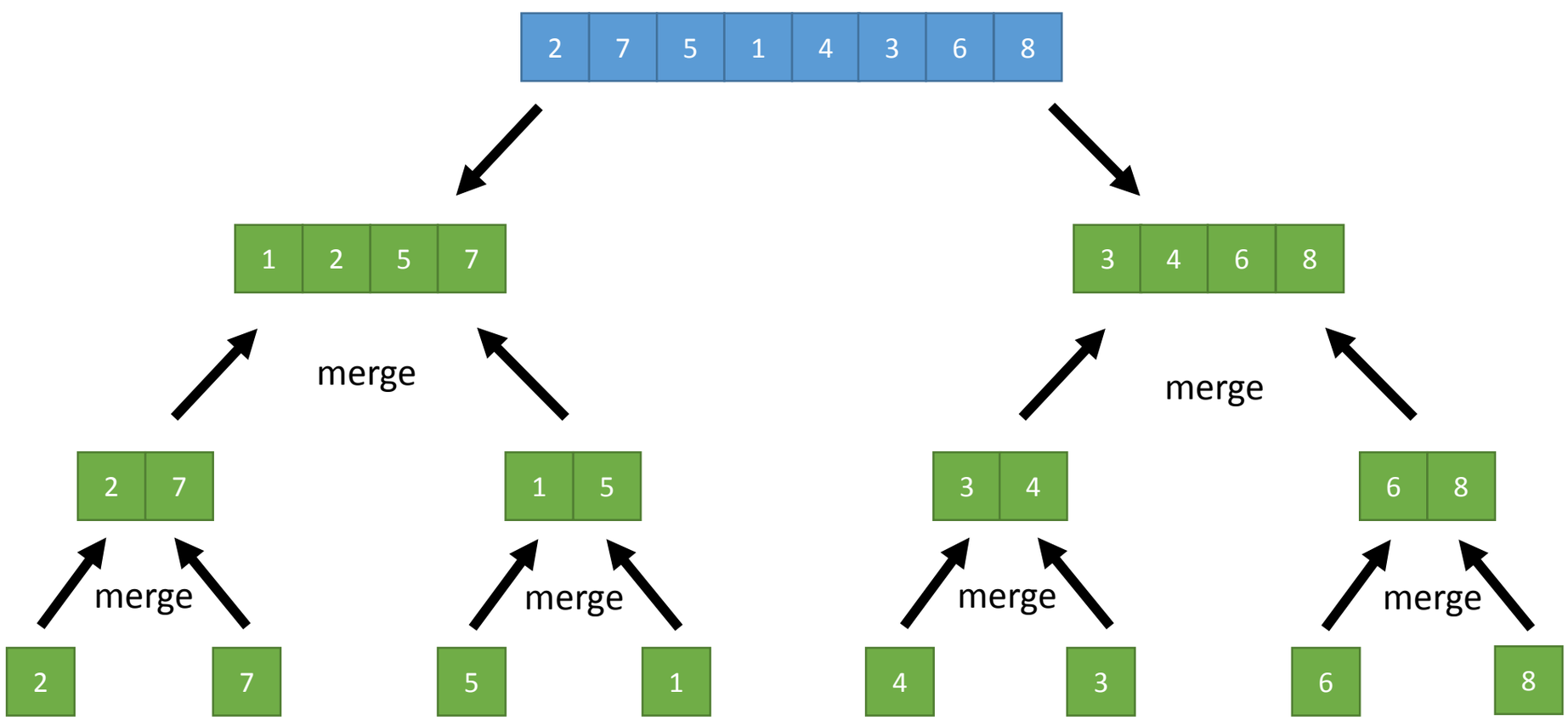
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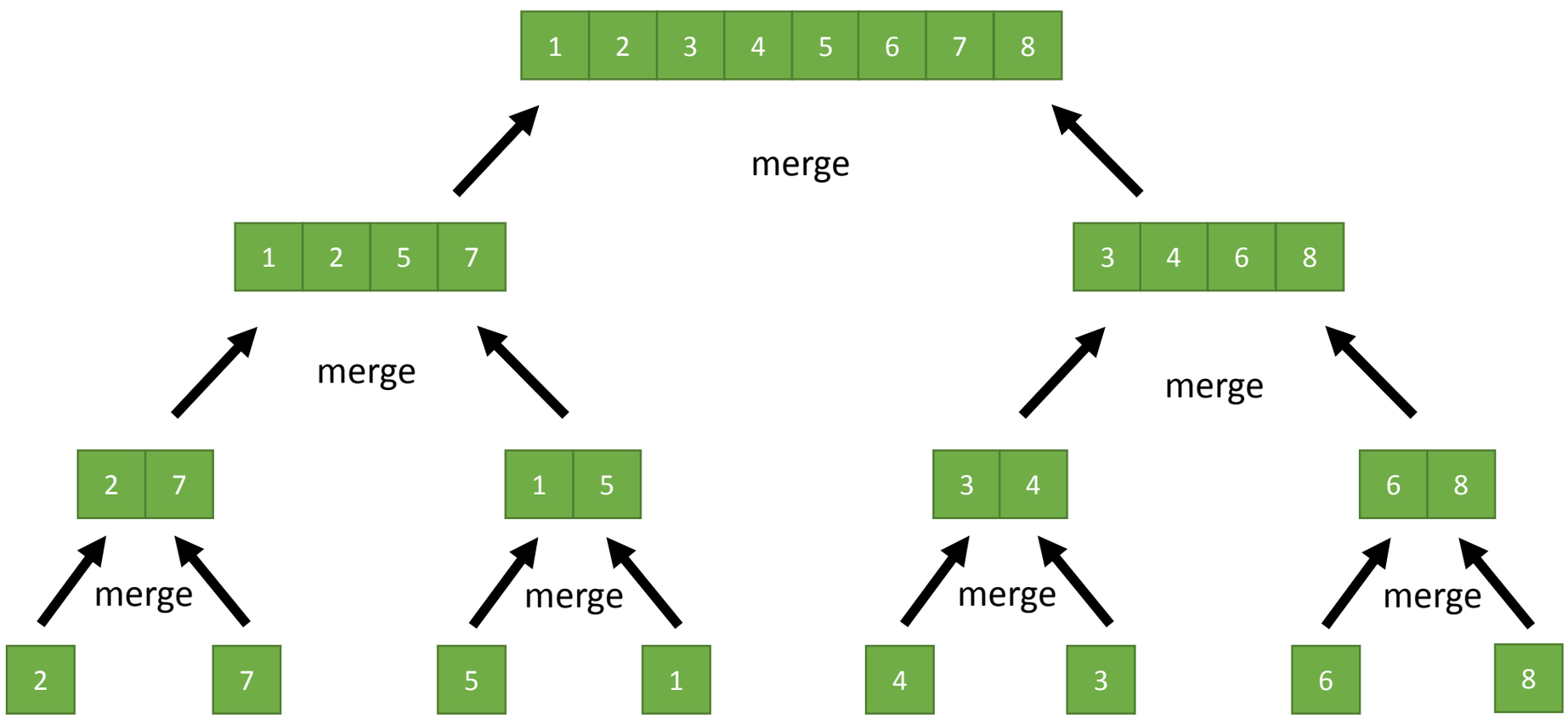
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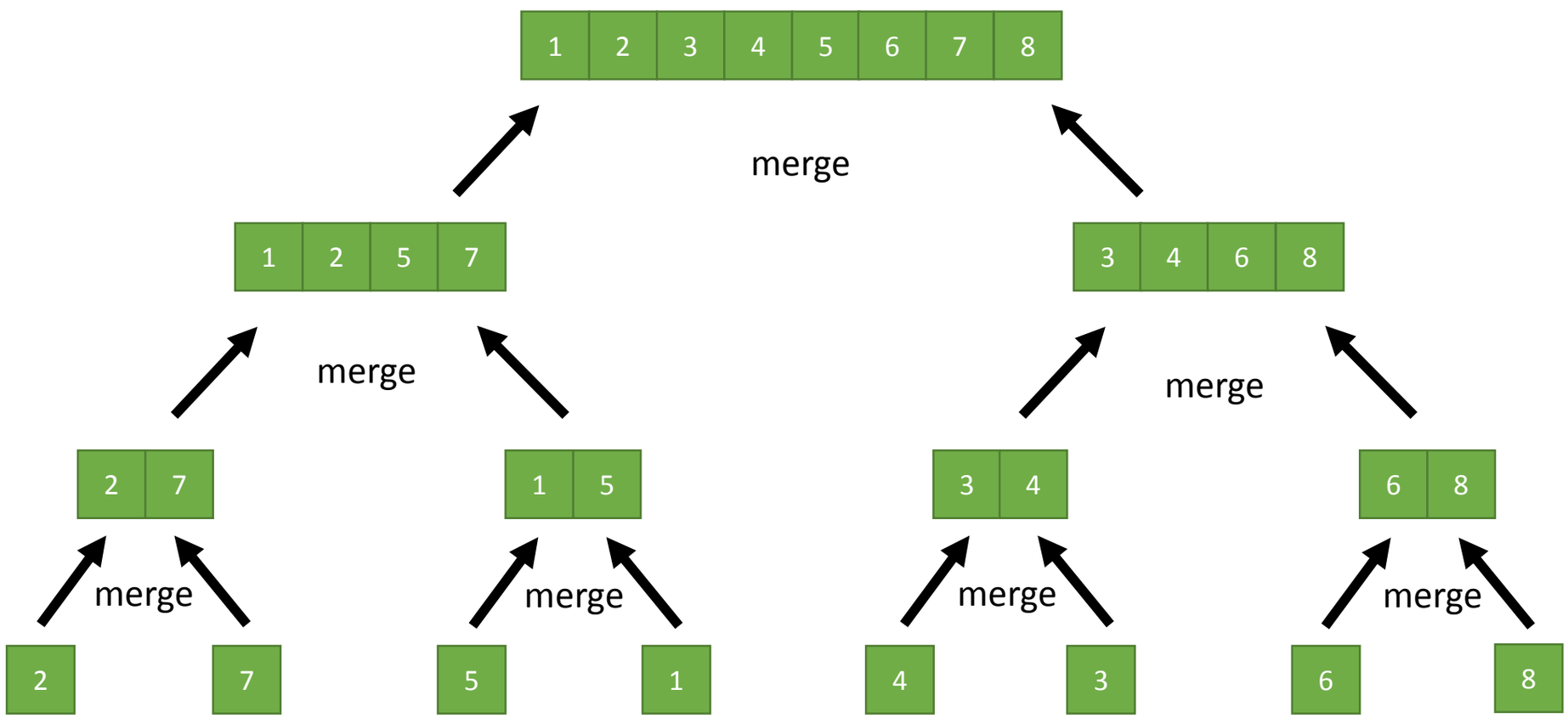
Merge Sort

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



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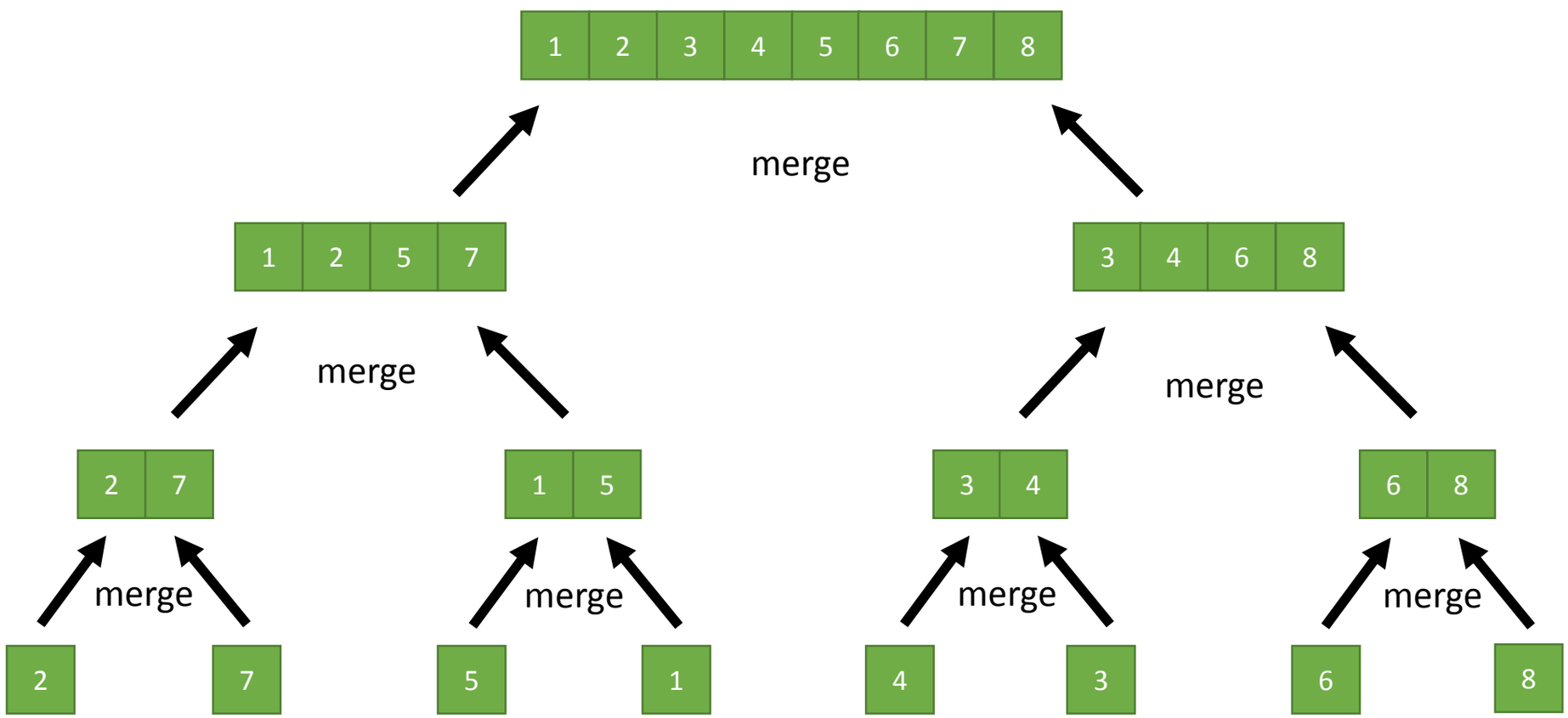

15 Sorting Algorithms in 6 Minutes

http://youtu.be/kPRA0W1kECg

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Data structure complexity

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http://bigocheatsheet.com/

Nicolai Josuttis, The C++ Standard Library.