

Optimization / Profiling

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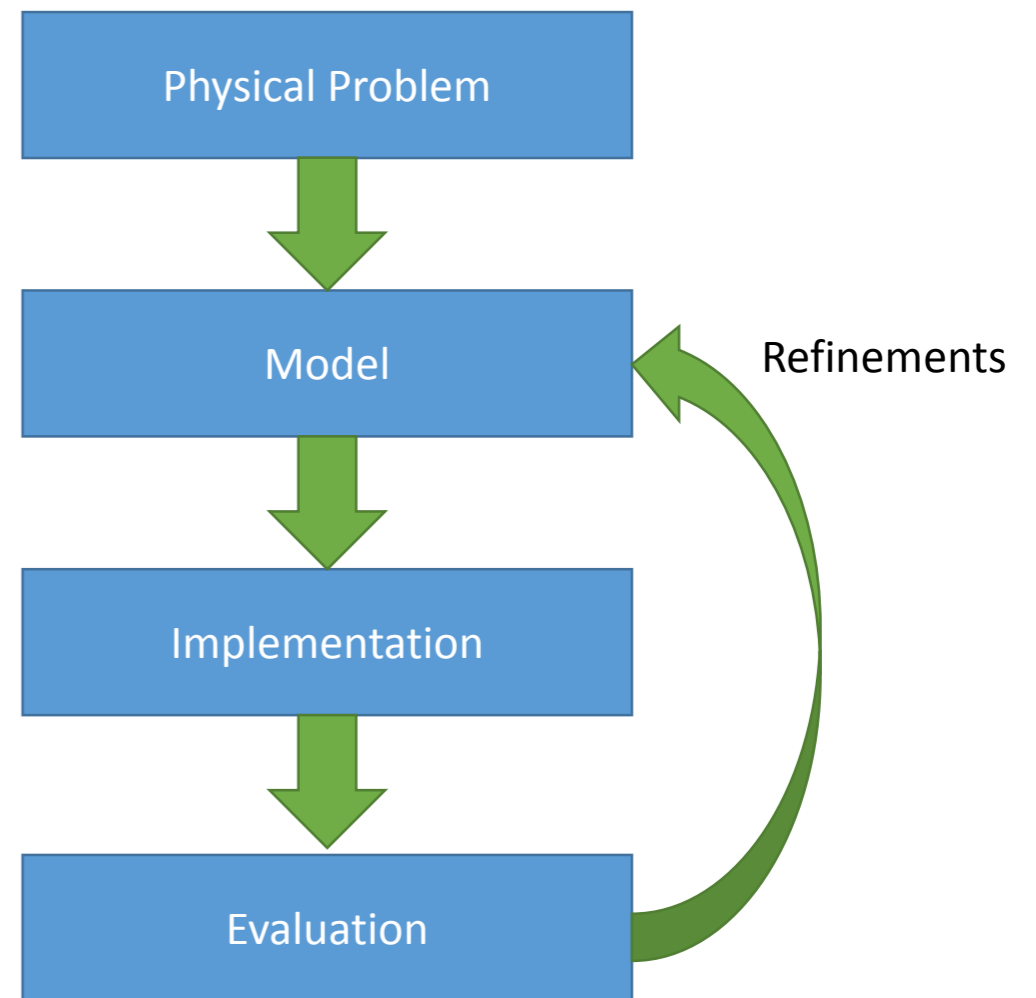
Typical scientific workflow

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)



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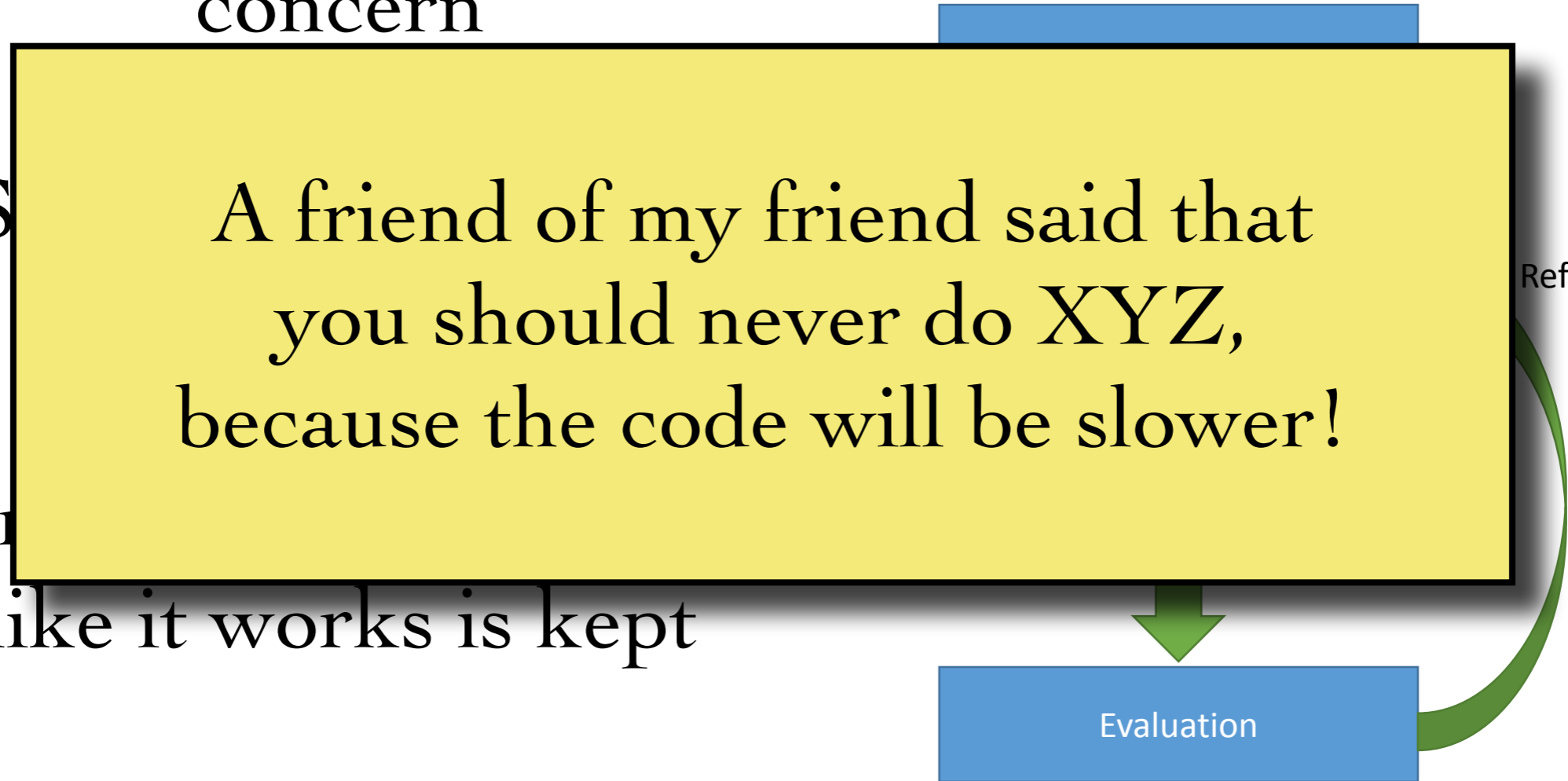
A friend of my friend said that
you should never do *XYZ*,
because the code will be slower!

Refinements

like it works is kept

Evaluation

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



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!

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

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

```
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 savings

Local and hardware-specific optimisations

- not in this course -

What are we optimizing?

Time

Memory

Disk

Electricity


Compile time

Ease of use

Ease of deployment

Ease of development

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Much simplified, skipping formal derivation

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while not is_sorted(xs):  
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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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Much simplified, skipping formal derivation

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```

$O(NN!)$

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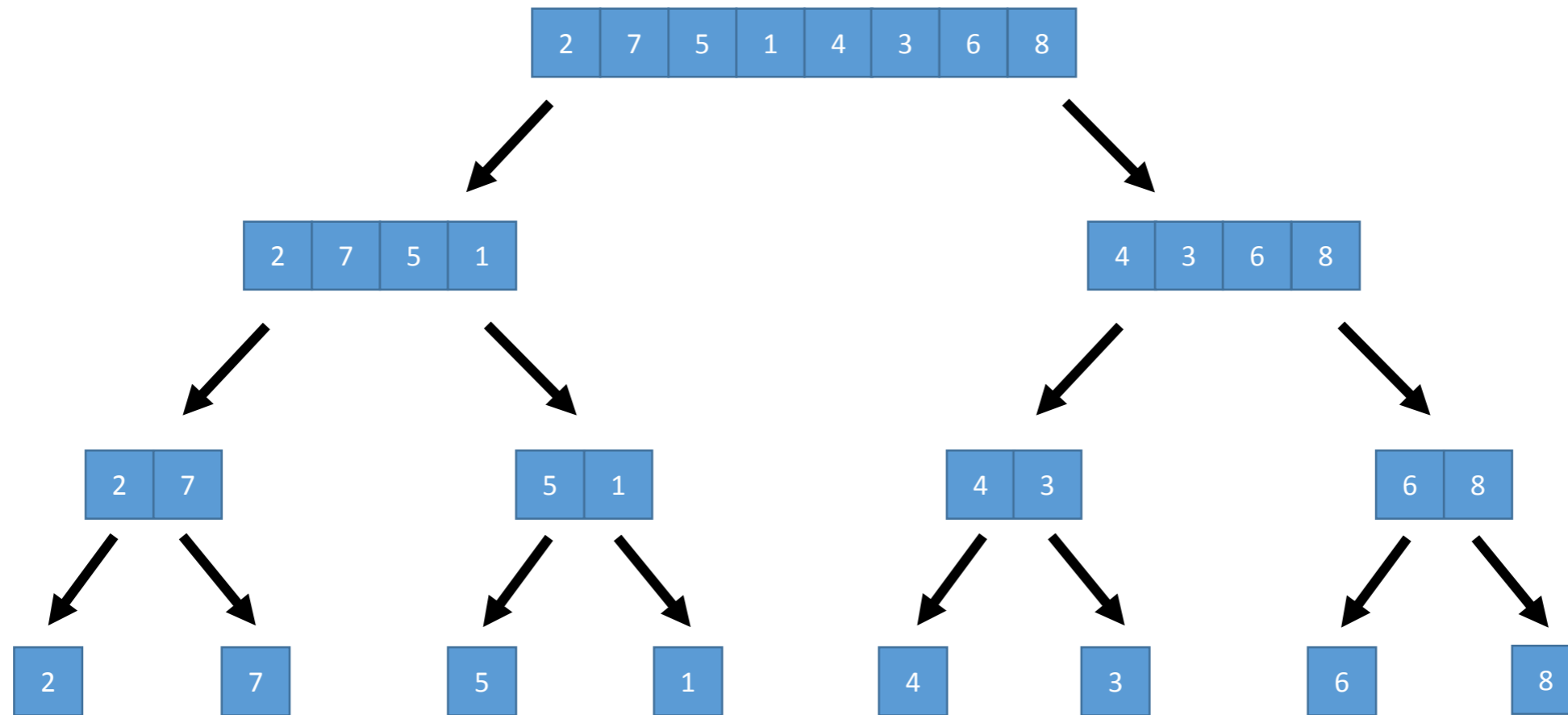
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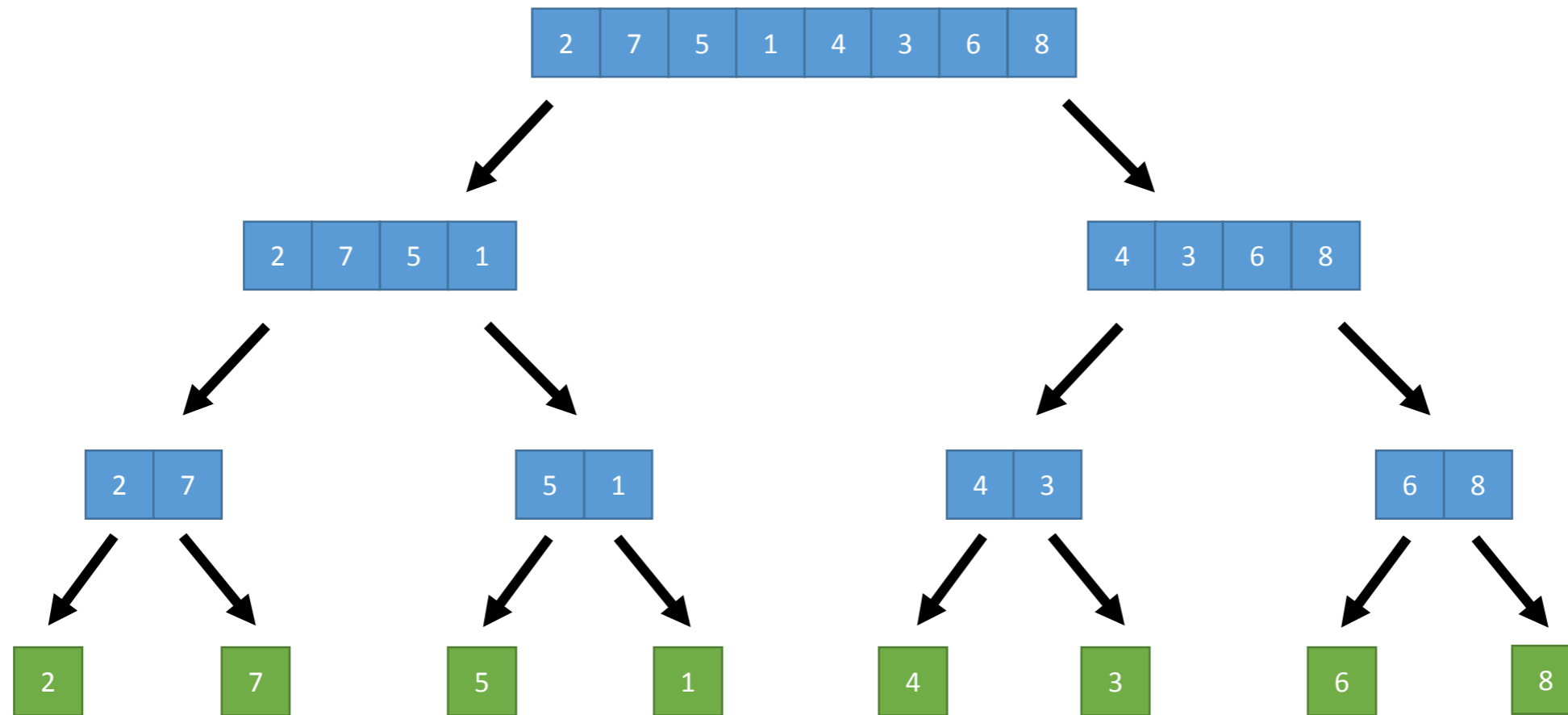
Merge Sort

2	7	5	1	4	3	6	8
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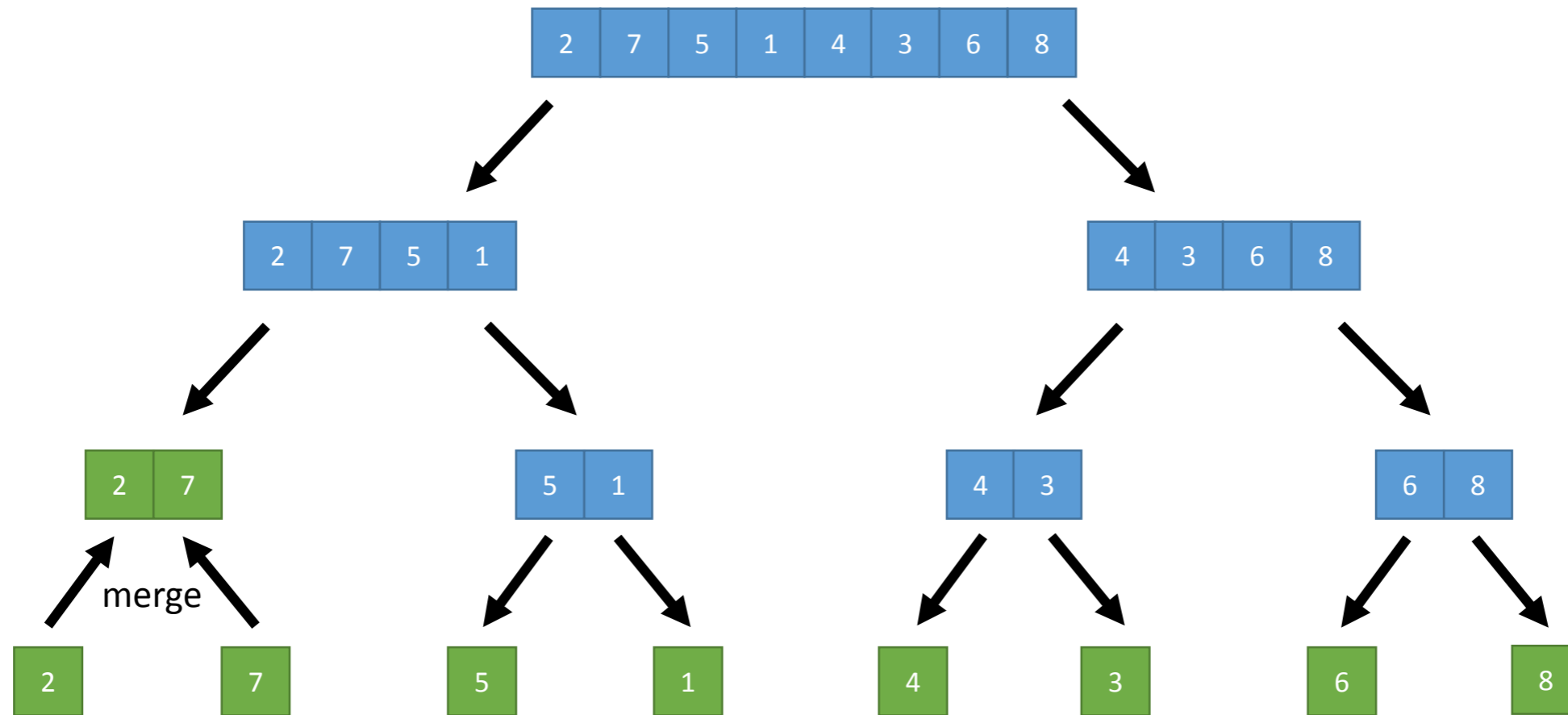
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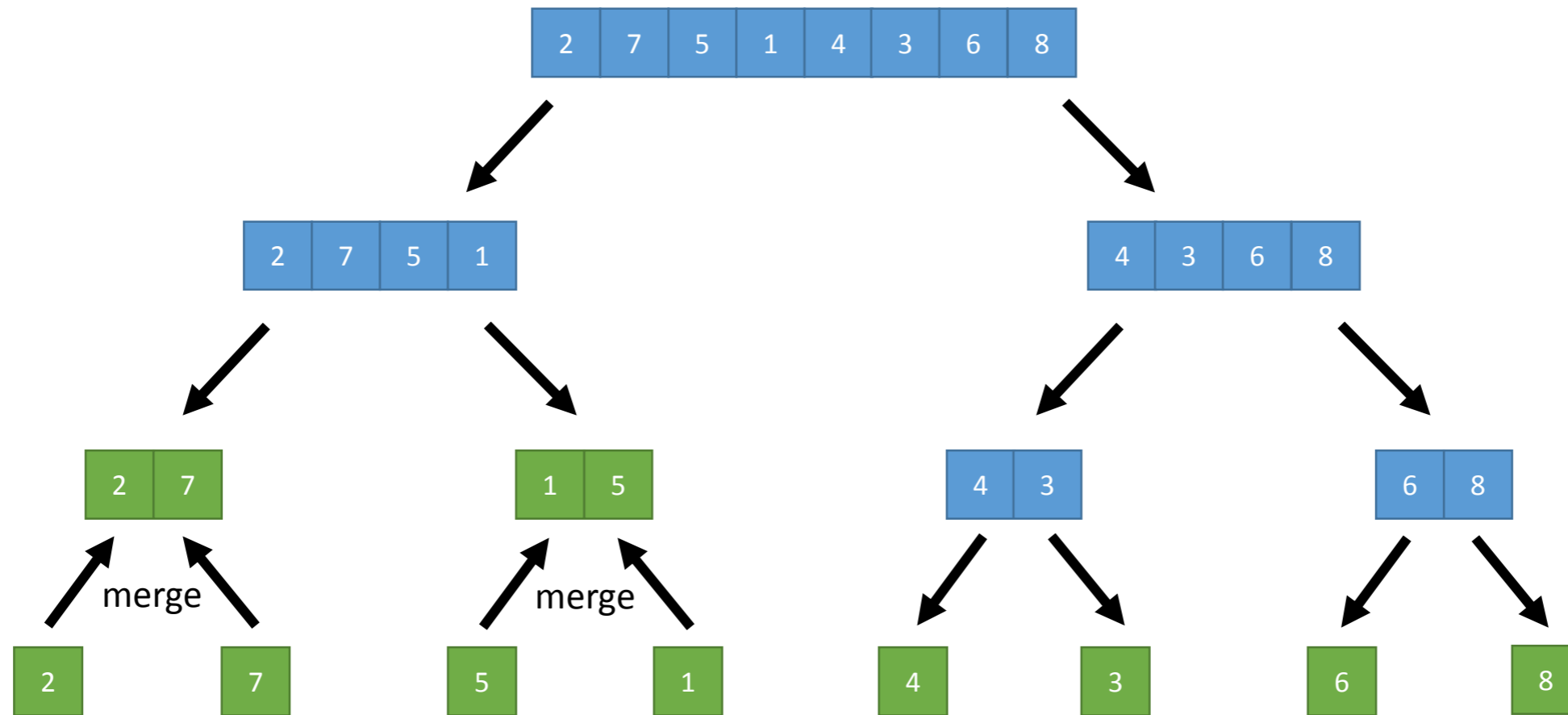
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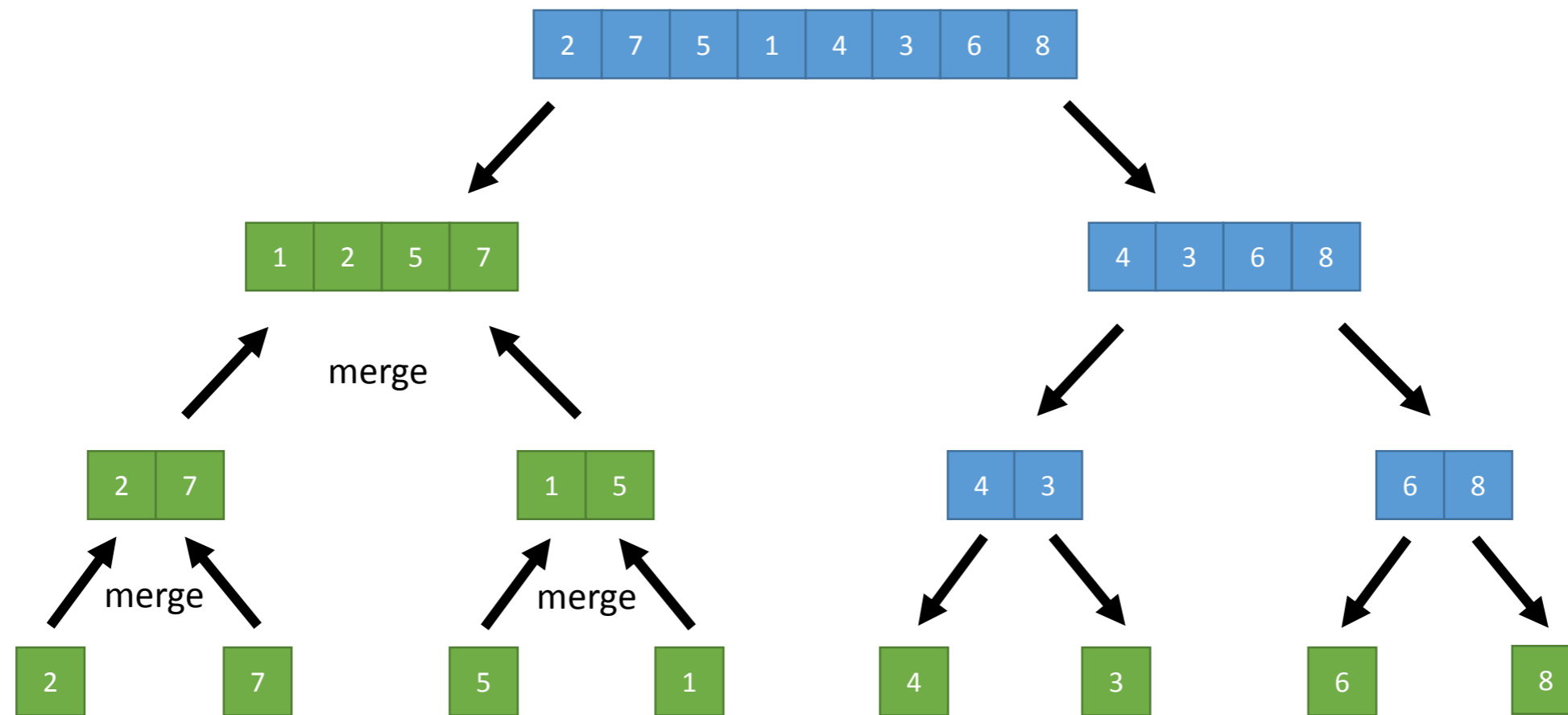
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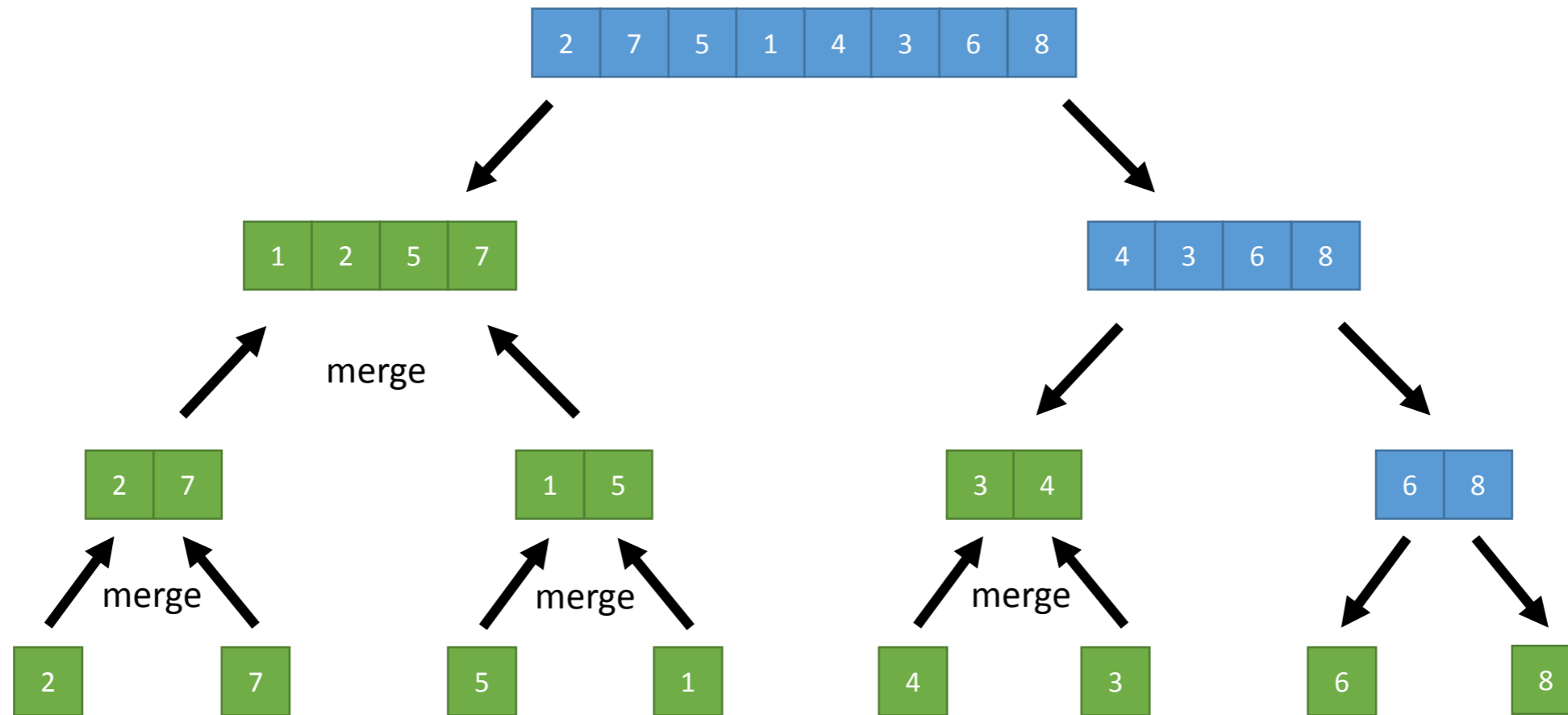
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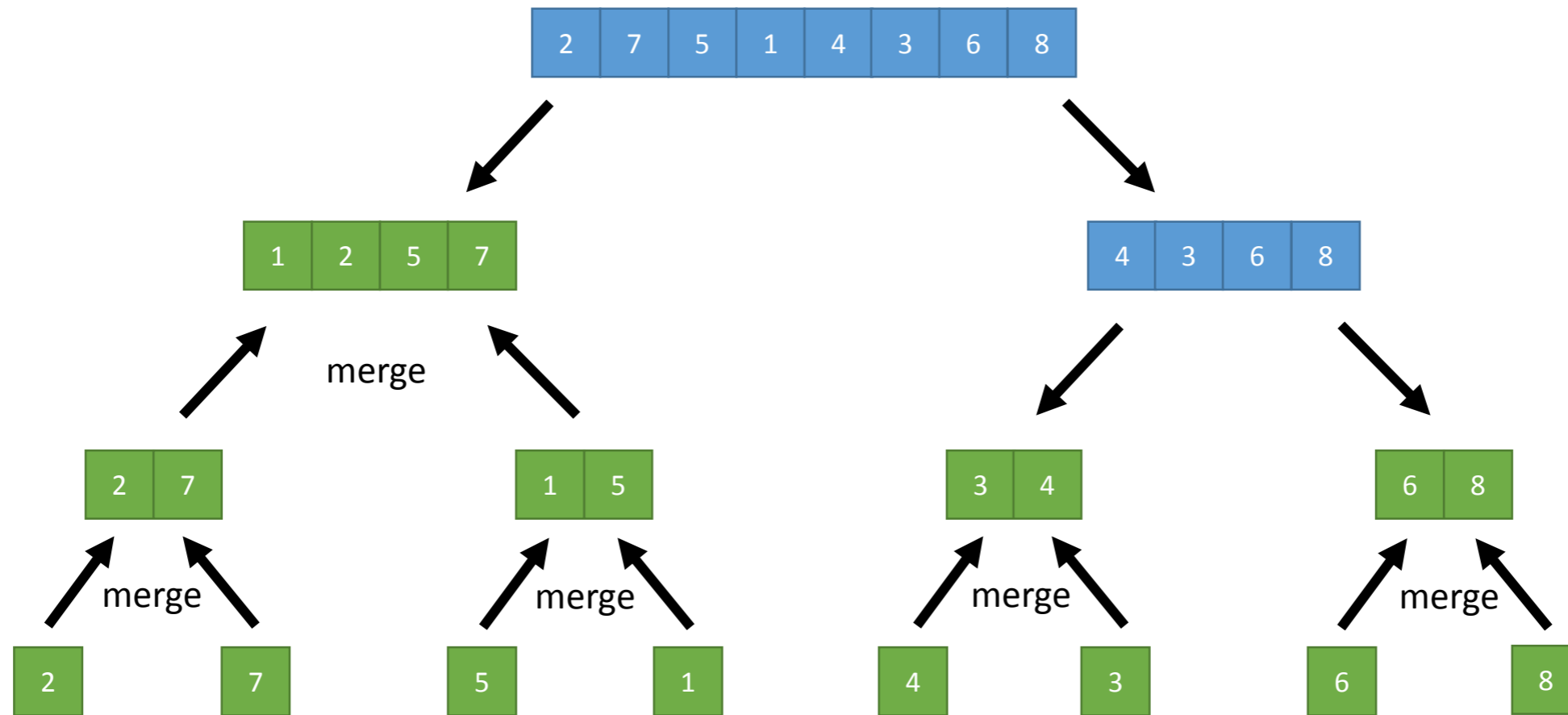
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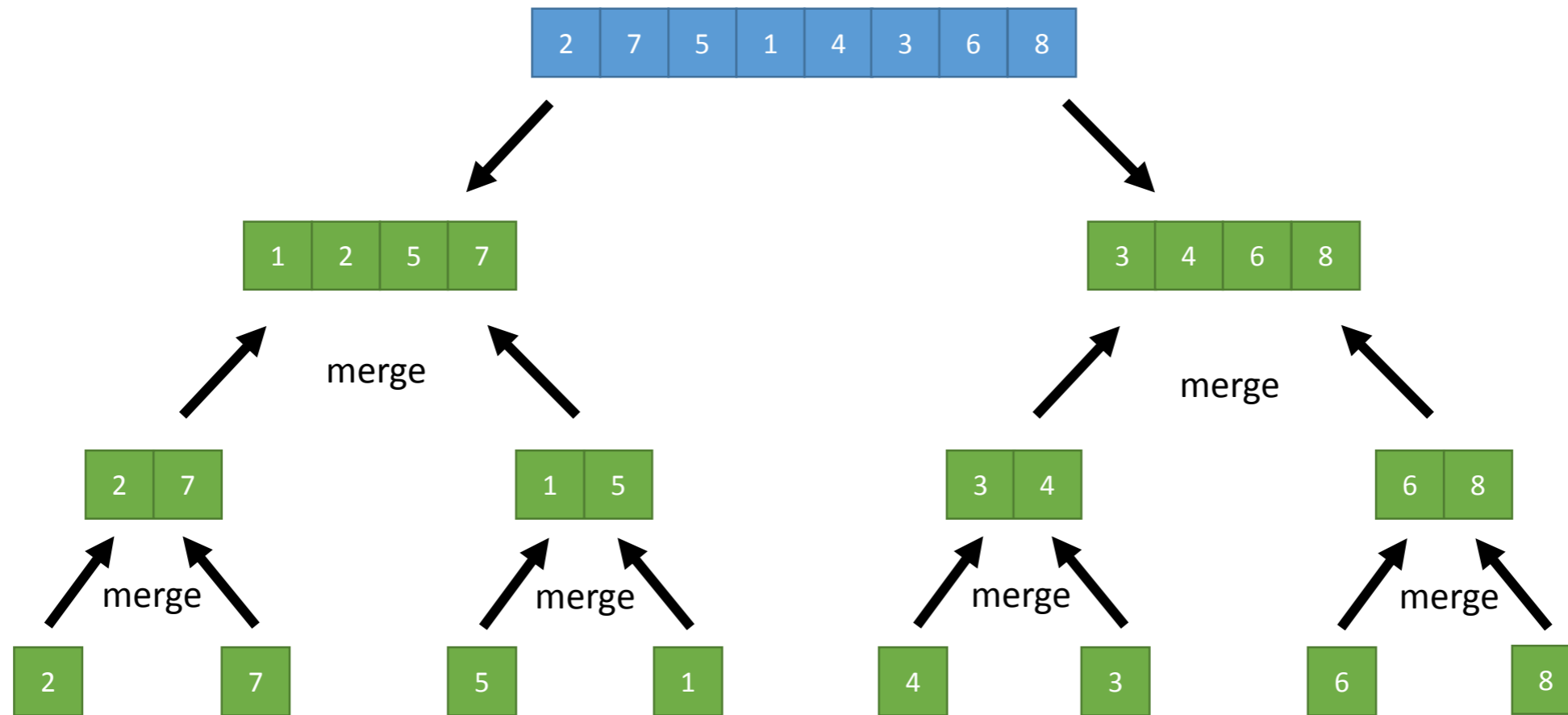
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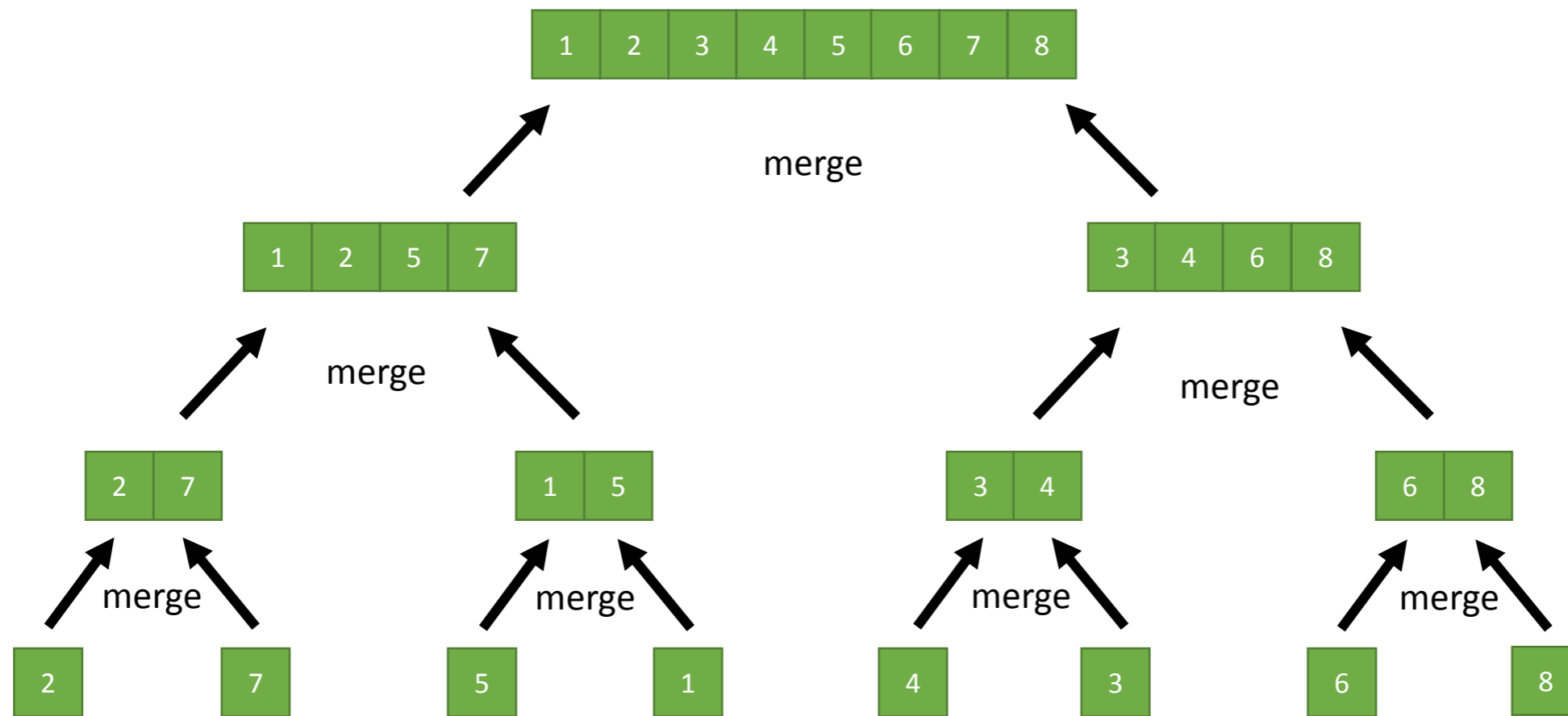
Merge Sort



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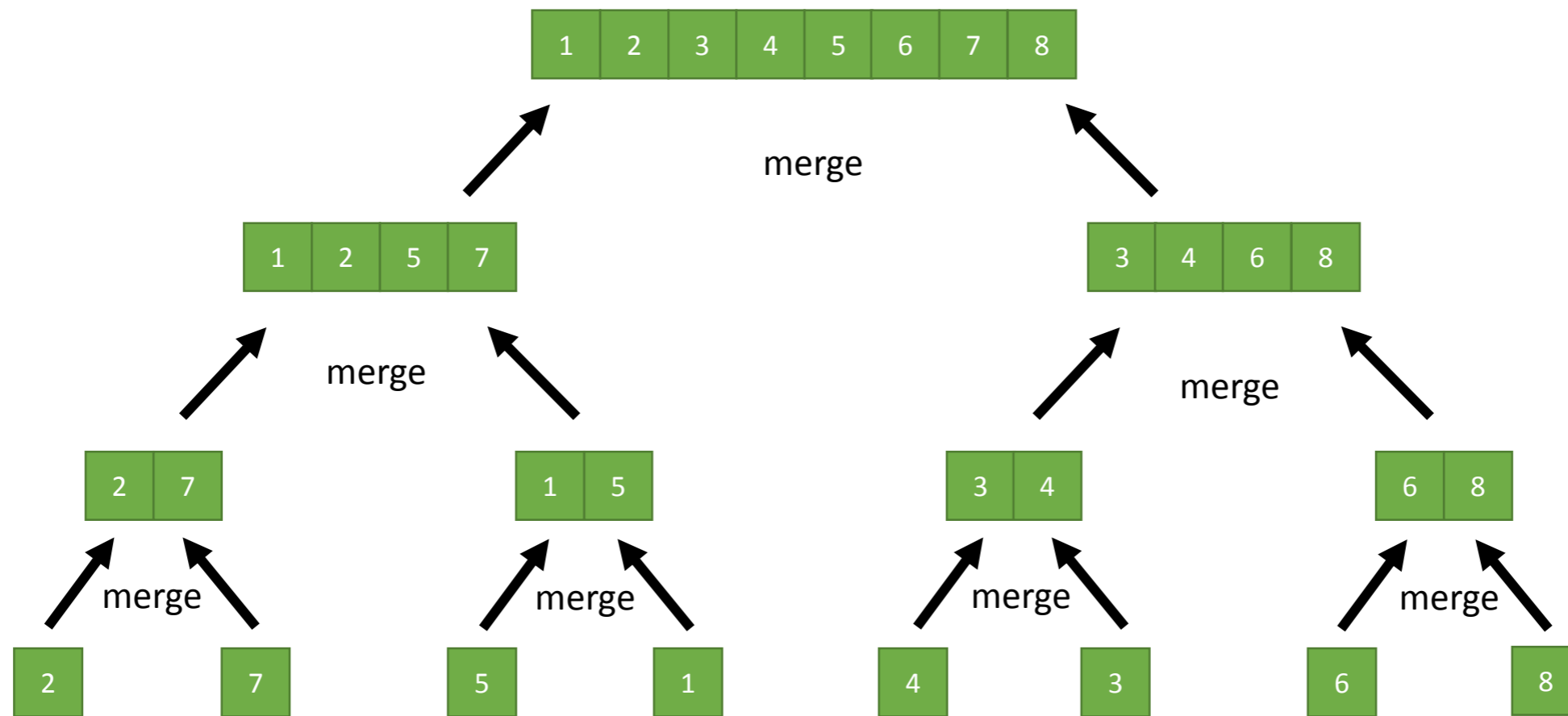


Merge Sort



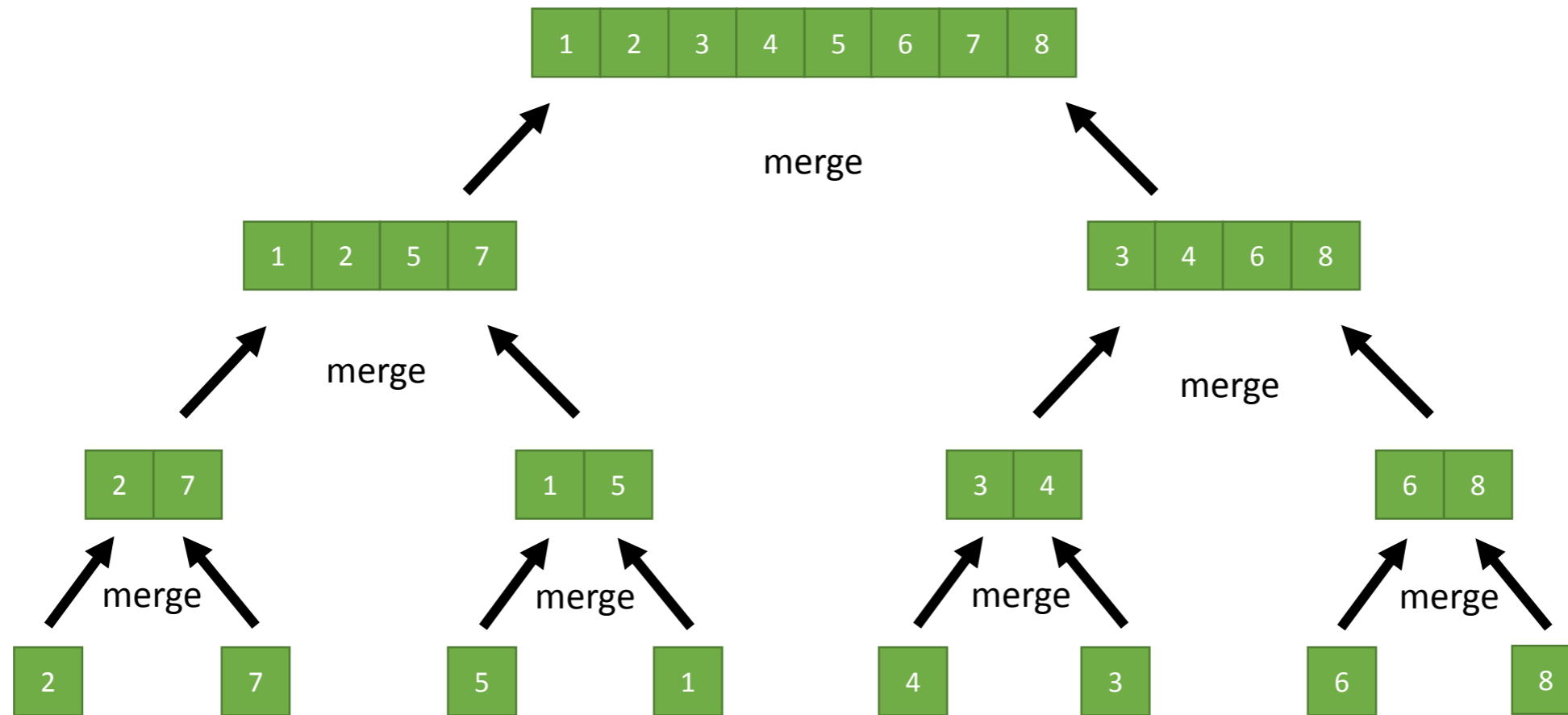
Merge Sort

$$O(N \log N)$$



Merge Sort

$$O(N \log N)$$



15 Sorting Algorithms in 6 Minutes

<http://youtu.be/kPRA0W1kECg>

Data structure complexity

Array
Vector

Linked list

Ordered map

Hash table

<http://bigocheatsheet.com/>

Nicolai Josuttis, “The C++ Standard Library”

Cache Memory

```
Loop: load r1, A(i)
      load r2, s
      mult r3, r2, r1
      store A(i), r2
      branch => loop
```

CPU
Registers

CACHE

MAIN MEMORY

- Designed for temporal/spatial locality
- Data is transferred to cache in blocks of fixed size, called *cache lines*.
- Operation of LOAD/STORE can lead at two different scenario:
 - *cache hit*
 - *cache miss*

LI cache reference 0.5 ns
Branch mispredict 5 ns
L2 cache reference 7 ns
Mutex lock/unlock 25 ns
Main memory reference 100 ns
SSD random read 150,000 ns = 150 μ s
Read 1 MB sequentially from memory 250,000 ns = 250 μ s
Read 1 MB sequentially from SSD 1,000,000 ns = 1 ms
Disk seek 10,000,000 ns = 10 ms
Read 1 MB sequentially from disk 20,000,000 ns = 20 ms
Send packet EU->US->EU 150,000,000 ns = 150 ms

L1 cache reference	0.5 s
Branch mispredict	5 s
L2 cache reference	7 s
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Main memory reference	100 s
SSD random read	1.7 days
Read 1 MB sequentially from memory	2.9 days
Read 1 MB sequentially from SSD	11.6 days

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Read 1 MB sequentially from SSD	11.6 days
Disk seek	16.5 weeks
Read 1 MB sequentially from disk	7.8 months

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Disk seek	16.5 weeks
Read 1 MB sequentially from disk	7.8 months
Send packet EU->US->EU	4.8 years

Optimization strategy

Don't optimize the whole code

Profile the code, find the bottlenecks

They may not always be where you thought they were

Break the problem down

Try to run the shortest possible test you can to get meaningful results

Isolate serial kernels

Keep a working version of the code!

Getting the wrong answer faster is not the goal.

Optimize on the architecture on which you intend to run

Optimizations for one architecture will not necessarily translate

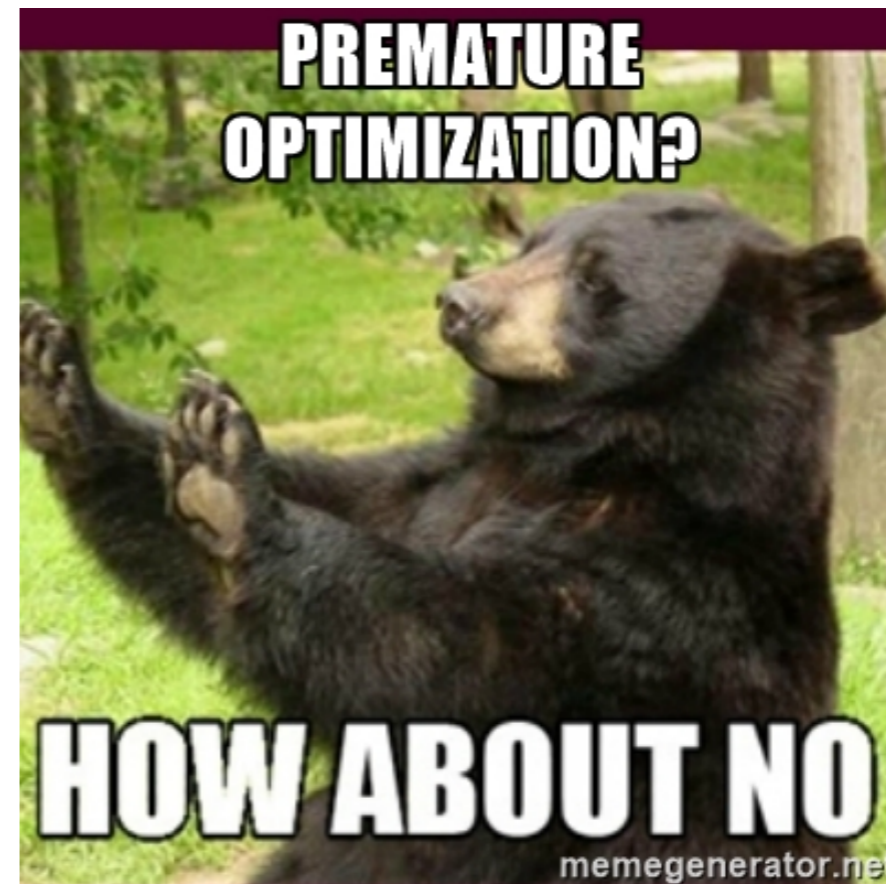
The compiler is your friend!

If you find yourself coding in machine language, you are doing too much.

This is the most important slide in the talk

Never, ever optimize unless you have good reason to.

- ▶ Why do you need to optimize?
- ▶ Do you have a clear plan of action?
- ▶ What do you expect to gain?
- ▶ How long will it take?
- ▶ Are you still sure it's worth it?



Python profiling options

time

```
from time import time
start = time()
somefunc(27)
end = time()
```

timeit

```
python -m timeit -s 'import myfile as m;'
x=27' 'm.somefunc(x)'
```

cProfile

```
import cProfile
cProfile.run(somefunc(27))
```

pyprof2calltree
qcachegrind

All are in the standard library

Link to compiled code

Try to stay with Python-only until performance becomes a problem. Numpy etc. make this possible

Interesting package to give just-in-time compilation on arbitrary code

<https://numba.pydata.org/>

Link to external code

ctypes for C (standard lib)

f2py for Fortran (part of numpy)

cython for C and C++ (on PyPI)

...