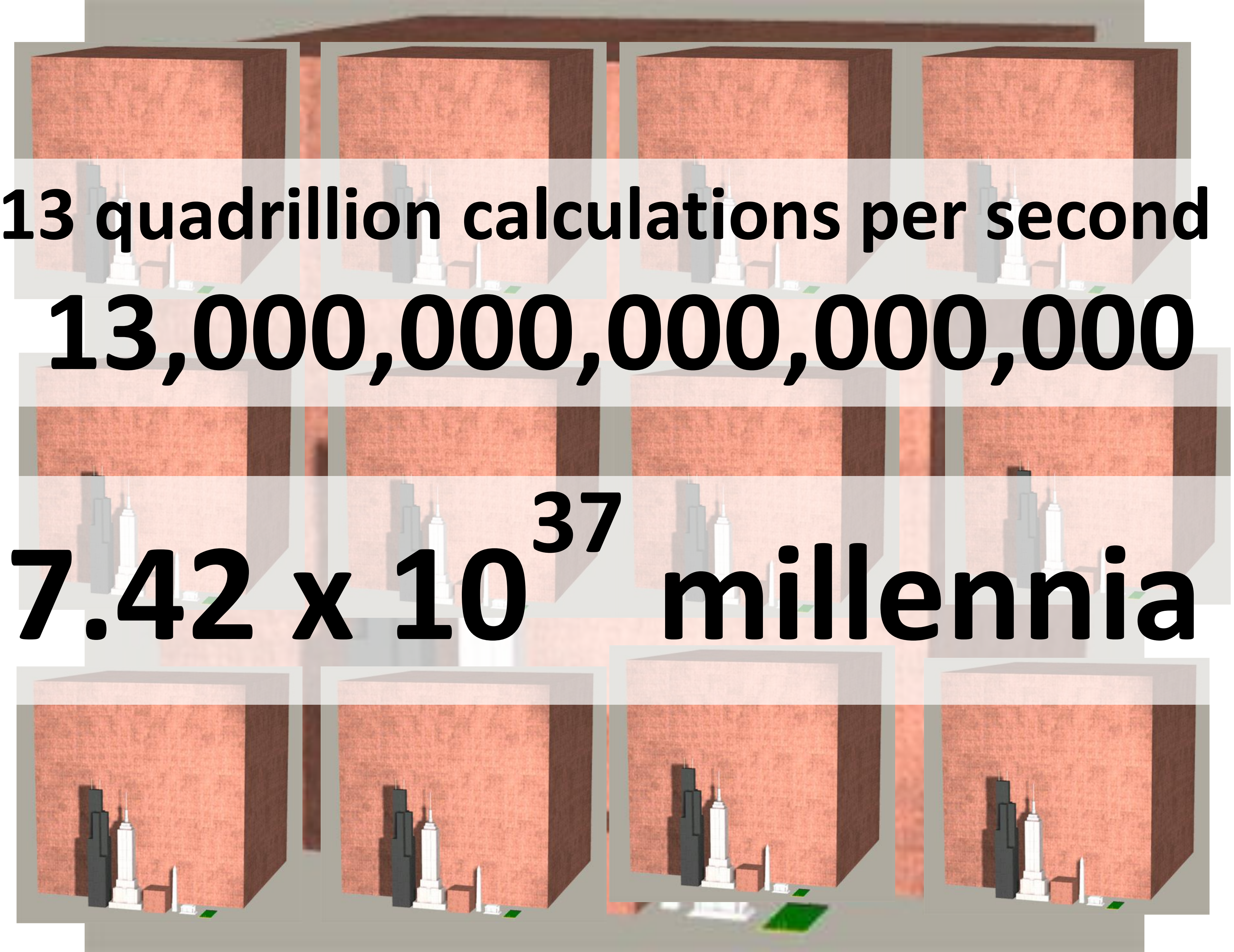
Algorithms and complexity (I)

Blue Waters

13 quadrillion calculations per second

13,000,000,000,000,000

http://www.ncsa.illinois.edu/enabling/bluewaters



13 quadrillion calculations per second

13,000,000,000,000,000

7.42×10^{37} millennia

An *algorithm* is a well-defined computational procedure that takes some values as input and produces some values as output.

Search a 1024 page dictionary to find which page the word “hippopotamus” is on.

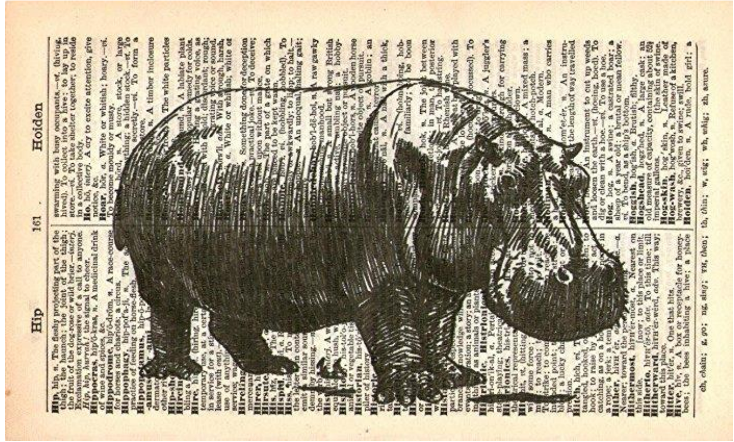
Option 1: start on page 1 and begin reading

Option 2: turn to middle, if word is before that page, it must be in first half; otherwise last half. Repeat.

1024/2→512/2→256/2→128/2→64/2→32/2→16/2→8/2→4/2→2/2→1

10 comparisons

Binary search



1. Algorithms help us to understand *scalability*
2. Algorithmic mathematics provides a *language* for talking about program behavior
3. Performance is the *currency* of computing

Performance often draws the line between ***what is feasible*** and ***what is impossible…***

1. **Correctness**
2. **Time Complexity**
3. **Space Complexity**

A (Correct, but Bad) Algorithm for the Assignment Problem:

Enumerate all possible assignments and choose the cheapest one.

E.g., assign members of set N1 to members of set N2

Let n = |N1| = |N2| Total: **n!** possible assignments

Suppose n = 70

70! =**1,978,571,669,969,891,796,072,783,721, 689,098,736,458,938,142,546,425,857,555, 362,864,628,009,582,789,845,319,680,000, 000,000,000,000**

Algorithms and complexity (II)

Theoretical Analysis

- Uses a high-level description of the algorithm instead of an implementation
- Characterizes running time as a function of the input size, n
- Takes into account all possible inputs
- Allows us to evaluate the speed of an algorithm independent of the hardware/software environment

Pseudocode

- High-level description of an algorithm
- More structured than English prose
- Less detailed than a program
- Hides program design issues
- Preferred notation for describing algorithms

Example: find max element of an array

Algorithm $\mathit{arrayMax}(A, n)$
  Input array A of n integers
  Output maximum element of A

  $\mathit{currentMax} \leftarrow A[0]$
  for $i \leftarrow 1$ **to** $n - 1$ **do**
    if $A[i] > \mathit{currentMax}$ **then**
      $\mathit{currentMax} \leftarrow A[i]$
  return $\mathit{currentMax}$

Each line shows one computation. Indentation is important

Algorithm 1 Adaboost (with Stump as the base learner)

Input: S: training set $\{(x(1),\ldots,x(N)\}$ with labels $\{y(1)\ldots,y(N)\}$
T: test set $\{u(1),u(2)\ldots u(N')\}$
K: number of rounds
Output: predictions $\{h(u_1),h(u_2)\ldots h(u_{N'})\}$ for all test instances.

```
For all i = 1 : N, w_1(i) = 1/N
for r = 1 to K do
   For all i = 1 : N, p_r(i) = w_r(i) / Σ_i (w_r(i))
   S_r = sampleByWeight(S, p_r, L), where L = N
   generate a new stump stp_r, call stp_r.learn(S_r)
   h_r^S = stp_r.classify(S)
   ε_r = Σ_i p_r(i) 1[h_r^S(i) ≠ y(i)]
   if ε_r > 1/2 or ε_r = 0 then
      K = r − 1
      Exit the loop
   end if
   β_r = ε_r / (1 − ε_r)
   For all i = 1 : N, w_{r+1}(i) = w_r(i) β_r^{1−1[h_r^S(i)≠y(i)]}
end for
For all r = 1 : K, h_r^T = stp_r.classify(T)
For all i = 1 : N', h(u_i) = arg max_{y∈Y} Σ_{r=1}^{K} log(1/β_r) 1[h_r^T(u_i) = y]
return {h(u_1), h(u_2) ... h(u_{N'})}
```

JOHNSON(G, w)

```
compute G′, where G′.V = G.V ∪ {s},
      G′.E = G.E ∪ {(s, v) : v ∈ G.V}, and
      w(s, v) = 0 for all v ∈ G.V
if BELLMAN-FORD(G′, w, s) == FALSE
      print "the input graph contains a negative-weight cycle"
else for each vertex v ∈ G′.V
           set h(v) to the value of δ(s, v)
                computed by the Bellman-Ford algorithm
      for each edge (u, v) ∈ G′.E
           ŵ(u, v) = w(u, v) + h(u) − h(v)
      let D = (d_uv) be a new n × n matrix
      for each vertex u ∈ G.V
           run DIJKSTRA(G, ŵ, u) to compute δ̂(u, v) for all v ∈ G.V
           for each vertex v ∈ G.V
                d_uv = δ̂(u, v) + h(v) − h(u)
urn D
```

lgorithm 2: Division

```
nction divide (x, y);
put: Two n-bit integers x and y, where y ≥ 1
utput: The quotient and remainder of x divided by y
x = 0 then
   return (q, r) = (0, 0)
se
   set (q, r) = divide(⌊x/2⌋, y);
   q = 2 × q, r = 2 × r;
   if x is odd then
      r = r + 1
   end
   if r ≥ y then
      r = r − y, q = q + 1
   end
   return (q, r)
```

Al
Re
En

```
      end if
   end for
   stepNo ←
end loop
```

SAT
form,
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edure

ical k-mer for x

```
      add x_rep to B
for all reads s do
   for all k-mers x in s do
      x_rep ← min(x, revcomp(x))
      if x_rep ∈ T then
         T[x_rep] ← T[x_rep] + 1
```

Control flow

- `if…then… [else …]`
- `while… do…`
- `repeat… until…`
- `for …do…`
- indentation replaces braces

Method declaration

Algorithm ***method*** **(*arg* [, *arg*…])** ← Name the procedure at the top

Input …

Output …

$\leftarrow$ assignment (similar to R)

$=$ equality testing (like "==")

Expressions

n^2 mathematical formulas and superscripts allowed

```
procedure iterated hill-climber
begin
   t ← 0
   initialize best
   repeat
   ...
   until t = MAX
end
```

```
procedure simulated annealing
begin
   ...
```

```
procedure tabu search
begin
   tries ← 0
   ...
   until tries = MA...
end
```

```
procedure evolutionary algorithm
begin
   t ← 0
   initialize P(t)
   evaluate P(t)
   while (not termination-condition) do
   begin
      t ← t + 1
      select P(t) from P(t − 1)
      alter P(t)
      evaluate P(t)
   end
end
```

Algorithm 3 NSGA-II algorithm

```
procedure NSGA-II(N′, g, f_k(x_k))     ▷ N′ members evolved g generations to solve f_k(x)
    Initialize Population ℙ′
    Generate random population - size N′
    Evaluate Objective Values
    Assign Rank (level) Based on Pareto dominance - sort
    Generate Child Population
      Binary Tournament Selection
      Recombination and Mutation
    for i = 1 to g do
        for each Parent and Child in Population do
            Assign Rank (level) based on Pareto - sort
            Generate sets of nondominated vectors along PF_known
            Loop (inside) by adding solutions to next generation starting from
the first front until N′ individuals found determine crowding distance between
points on each front
        end for
        Select points (elitist) on the lower front (with lower rank) and are outside
a crowding distance
        Create next generation
            Binary Tournament Selection
            Recombination and Mutation
    end for
end procedure
```

Algorithms and complexity (III)

Theoretical Analysis

- Uses a high-level description of the algorithm instead of an implementation
- Characterizes running time as a function of the input size, n
- Takes into account all possible inputs
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primitive operations

- Basic computations performed by an algorithm
- Largely independent from the programming language
- Exact definition not important
- Assumed to take a constant amount of time

Examples:

- **Evaluating an expression**
- **Assigning a value to a variable**
- **Indexing into an array**
- **Calling a method**
- **Returning from a method**

Can count the primitive operations:

Algorithm $arrayMax(A, n)$	# operations
$currentMax \leftarrow A[0]$	2
for $i \leftarrow 1$ **to** $n - 1$ **do**	$2 + n$
if $A[i] > currentMax$ **then**	$2(n - 1)$
$currentMax \leftarrow A[i]$	$2(n - 1)$
{ increment counter i }	$2(n - 1)$
return $currentMax$	1

Add 'em up and get the total: Total $7n - 1$

Define: Define the bounds of the operations

a = time taken by the fastest primitive operation

b = time taken by the slowest primitive operation

Let *T*(*n*) be *worst-case time* of *arrayMax*

Then: $\boldsymbol{a(7n - 1) \leq T(n) \leq b(7n - 1)}$

Hence, the running time *T*(*n*) is bounded by two *linear functions*.

The linear growth rate of the running time $T(n)$ is an intrinsic property of algorithm *arrayMax*

Write an algorithm using pseudocode that reads a positive integer N and calculates the sum of all integers 1..N,

i.e., $1 + 2 + \ldots + N = ?$

EXAMPLE OF ALGORITHM VIA PSEUDO-CODE

Algorithm Name: **Sum** (N)

Input: integer $N \geq 0$

Output: sum of integers 1 to N

	<u># of operations</u>
$total \leftarrow 0$	1
for $i \leftarrow 1$ to N do	3+N
$\quad total \leftarrow total + i$	2N
	(increment counter) N
return *total*	1

Algorithm Name: **Sum** (N)

Input: integer $N \geq 0$

Output: sum of integers 1 to N

	<u># of operations</u>
$total \leftarrow \frac{N\,(N+1)}{2}$	4
return *total*	1

Algorithms and complexity (IV)

Theoretical Analysis

- Uses a high-level description of the algorithm instead of an implementation
- Characterizes running time as a function of the input size, *n*
- Takes into account all possible inputs
- Allows us to evaluate the speed of an algorithm independent of the hardware/software environment

Worst-case: (usually)

$T(n)$ =maximum time of algorithm on any input of size n

Average-case: (sometimes)

$T(n)$ =expected time of algorithm over all inputs of size n

Need assumption of statistical distribution of inputs

Best-case: (bogus)

Cheat with a slow algorithm that works fast on *some* input

Example: the problem of sorting

Input: sequence $\langle a_1, a_2, \ldots, a_n \rangle$ of numbers.

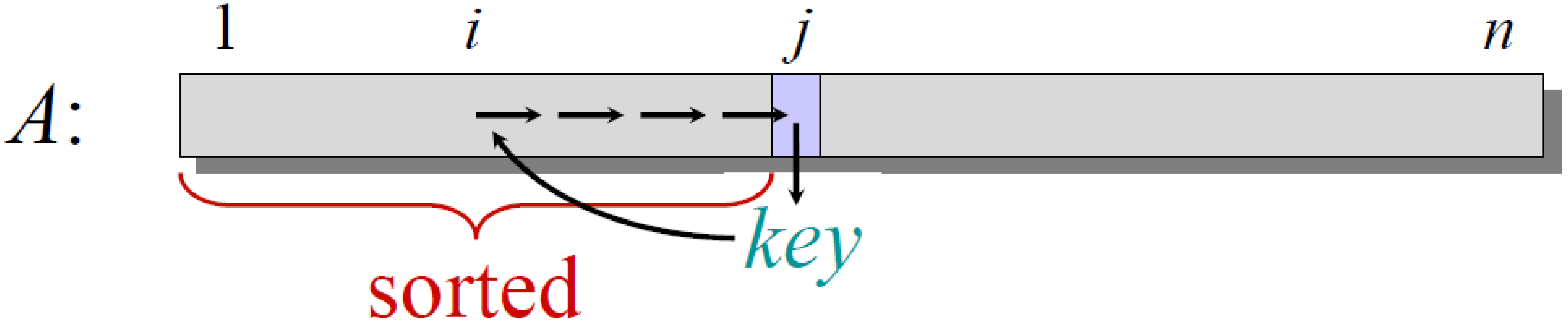
Output: permutation $\langle a'_1, a'_2, \ldots, a'_n \rangle$ such that $a'_1 \le a'_2 \le \cdots \le a'_n$.

Example:

Input: 8 2 4 9 3 6

Output: 2 3 4 6 8 9

```
INSERTION-SORT (A, n)
  for j ← 2 to n
      do key ← A[ j]
         i ← j – 1
         while i > 0 and A[i] > key
             do A[i+1] ← A[i]
                i ← i – 1
         A[i + 1] ← key
```



8 2 4 9 3 6

2 8 4 9 3 6

j=2

key = A[j] = A[2] = 2

i=j-1=1

A[i] = A[1]=8 > key =2

so, A[i+1] ← A[i]

A[2] ←A[1] = 8

i ← i-1 =0 A[i+1]=A[0+1]=A[1] ← key = 2

INSERTION-SORT (A, n) $\triangleright A[1 \,..\, n]$

for $j \leftarrow 2$ **to** n

do $key \leftarrow A[j]$

$i \leftarrow j - 1$

while $i > 0$ and $A[i] > key$

do $A[i+1] \leftarrow A[i]$

$i \leftarrow i - 1$

$A[i+1] = key$

8 2 4 9 3 6

2 8 4 9 3 6

j=3; key = A[j] = A[3] = 4; i=j-1=2

A[i] = A[2]=8 > key =4

so, A[i+1] ← A[i]

A[3] ←A[2] = 8

i ← i-1 =1

A[i] = A[1

so, end w

A[i+1]=A[

```
INSERTION-SORT (A, n)      ⊳ A[1 . . n]
  for j ← 2 to n
       do key ← A[ j]
          i ← j – 1
          while i > 0 and A[i] > key
               do A[i+1] ← A[i]
                  i ← i – 1
          A[i+1] = key
```

8 2 4 9 3 6

2 8 4 9 3 6

2 4 8 9

running time

- ~~Running time depends on the input: e.g., an already sorted sequence is easier to sort~~ **Usually: worst-case!**
- Parameterize the running time by the *size of the input*, e.g. short sequen … than long ones
- Generally, we seek … ing time, because everyboo
- Speed of computer

```
INSERTION-SORT (A, n)        ▷ A[1 . . n]
    for j ← 2 to n
        do key ← A[j]
           i ← j – 1
           while i > 0 and A[i] > key
               do A[i+1] ← A[i]
                  i ← i – 1
           A[i+1] = key
```

Algorithms and complexity (V)

Theoretical Analysis

- Uses a high-level description of the algorithm instead of an implementation
- Characterizes running time as a function of the input size, n
- Takes into account all possible inputs
- Allows us to evaluate the speed of an algorithm independent of the hardware/software environment

What is insertion sort's worst-case time?

- It depends on the speed of our computer:
  - relative speed (on the same machine)
  - absolute speed (on different machines)

BIG IDEA:

- Ignore machine-dependent constants.
- Look at *growth* of $T(n)$ as $n \to \infty$

"Asymptotic Analysis"

```
INSERTION-SORT (A, n)
    for j ← 2 to n
        do key ← A[j]
           i ← j – 1
           while i > 0 and A[i] > key
               do A[i+1] ← A[i]
                  i ← i – 1
           A[i+1] = key
```

$$T(n) = \frac{1}{2}p\left(n^2 - n\right) \qquad \text{for some } 1 \leq p \leq P$$

$$\frac{1}{2}\left(n^2 - n\right) \leq T(n) \leq \frac{1}{2}P\left(n^2 - n\right)$$

Pro-tip: ***constants and lower-order terms don't matter***

“Big O” notation describes the asymptotic upper bound of an algorithms growth rate

$$T(n) \in \mathcal{O}\left(f(n)\right)$$

The asymptotic lower bound on growth rates is expressed by “Big Omega “ notation

$$T(n) \in \Omega\left(f(n)\right)$$

If the upper and lower bounds are the same, “Big Theta”

$$T(n) \in \Theta\left(f(n)\right)$$

$$T(n) \in \mathcal{O}\left(f(n)\right)$$

$$\text{iff } \exists N \geq 0, c > 0,$$

$$T(n) \leq c f(n) \ \forall n \geq N$$

$$T(n) \in \mathcal{O}\left(f(n)\right) \text{ iff } \exists N \geq 0, c > 0,$$
$$T(n) \leq cf(n)\ \forall n \geq N$$

Examples:

One possible set of values

$$T(n) = 0.01n^3 \in \mathcal{O}(n^3)$$

$c = 0.02; N = 0;$

$T(n) \leq 0.02n^3\ \forall n \geq 0$

$$T(n) = 6n^2 + 10n + 7 \in \mathcal{O}(n^2)$$

$c = 10;\ N = 4$

$T(n) \leq 10n^2\ \forall n \geq 4$

$$T(n) = n^3 + 10^6 n^2 \in \mathcal{O}(n^3)$$

$c = 10;\ N = 112{,}000$

$T(n) \leq 10n^3\ \forall n \geq 112000$

Many upper bounds exist…

$$T(n) = n^2 \in \mathcal{O}(n^2), \mathcal{O}(n^3), \ldots, \mathcal{O}(n^{100}), \ldots$$

Note: usually when people talk about Big-O, they normally talking about the smallest upper bound

$T(n) \in \mathcal{O}\left(f(n)\right)$ iff $\exists N \geq 0, c > 0,$
$T(n) \leq cf(n)\ \forall n \geq N$

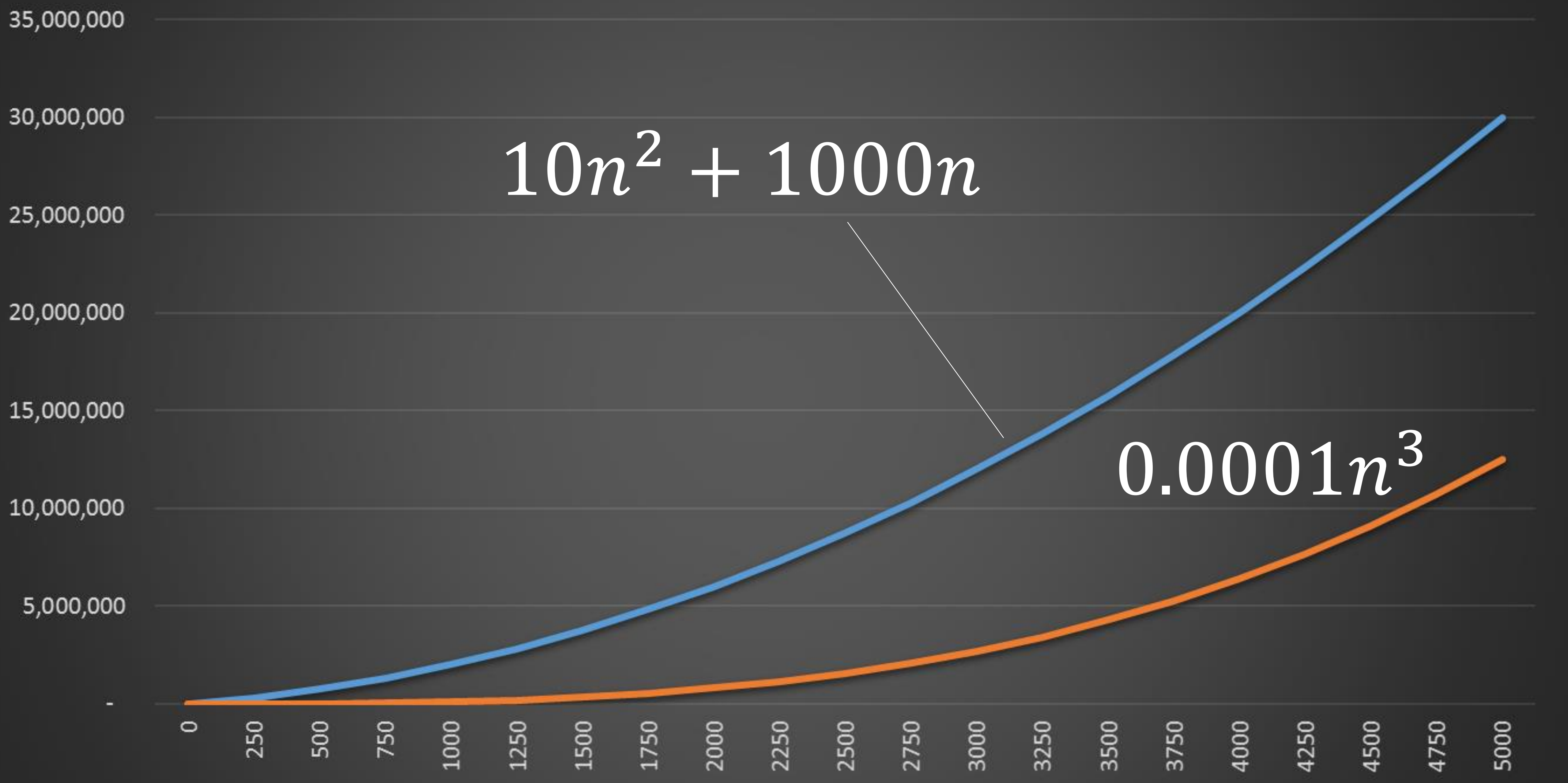
More examples:

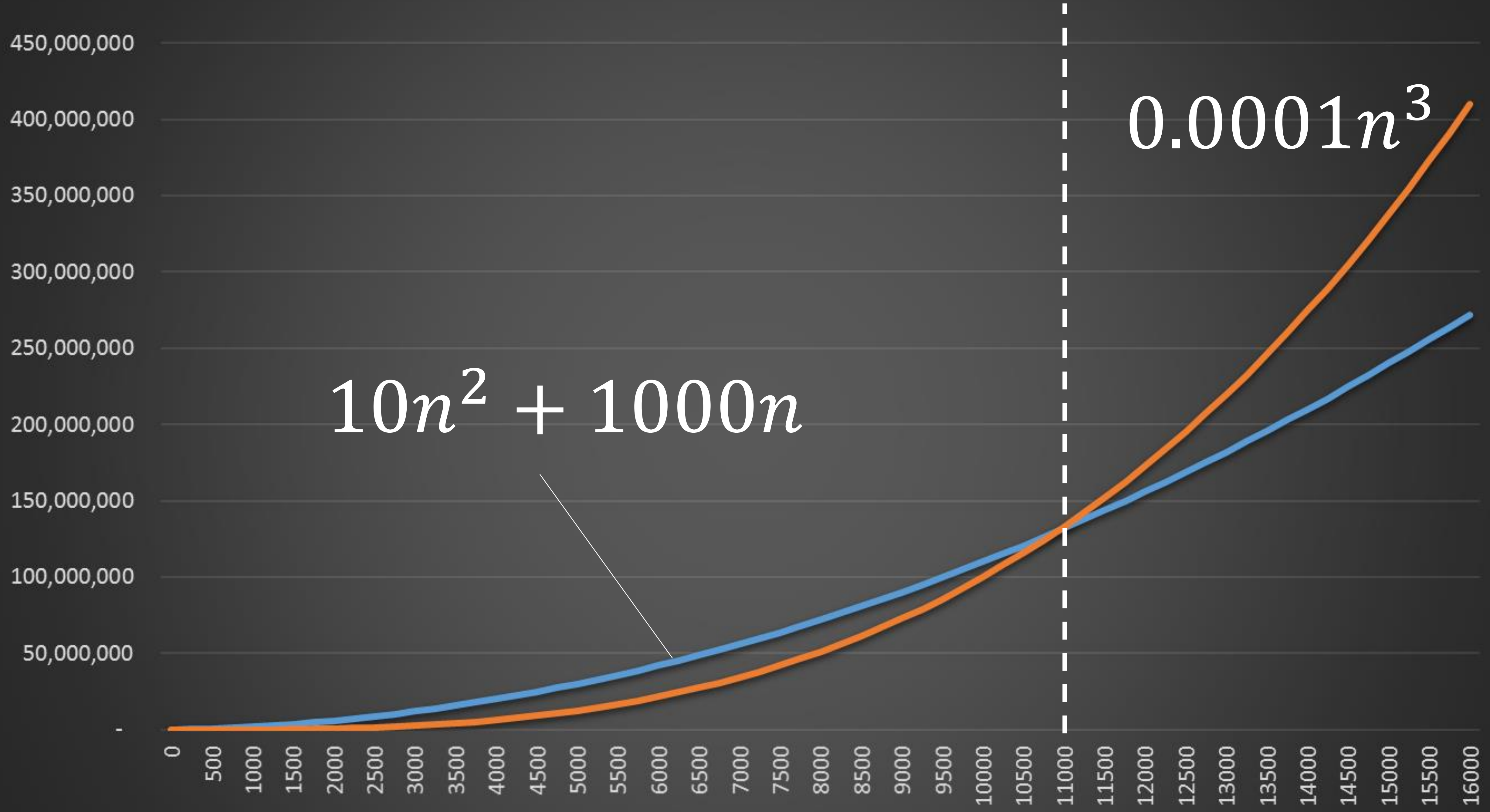
$$0.0001n^3 \notin \mathcal{O}(n) \qquad 10n^2 + 1000n \notin \mathcal{O}(n)$$

$$0.0001n^3 \notin \mathcal{O}(n^2) \qquad 10n^2 + 1000n \in \mathcal{O}(n^2)$$

$$0.0001n^3 \in \mathcal{O}(n^3) \qquad 10n^2 + 1000n \in \mathcal{O}(n^3)$$

$$0.0001n^3 \in \mathcal{O}(n^4) \qquad 10n^2 + 1000n \in \mathcal{O}(n^4)$$


35,000,000
30,000,000
25,000,000
20,000,000
15,000,000
10,000,000
5,000,000
-
0
250
500
750
1000
1250
1500
1750
2000
2250
2500
2750
3000
3250
3500
3750
4000
4250
4500
4750
5000
$10n^2 + 1000n$
$0.0001n^3$


$0.0001n^3$
$10n^2 + 1000n$
450,000,000
400,000,000
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250,000,000
200,000,000
150,000,000
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7000
7500
8000
8500
9000
9500
10000
10500
11000
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16000

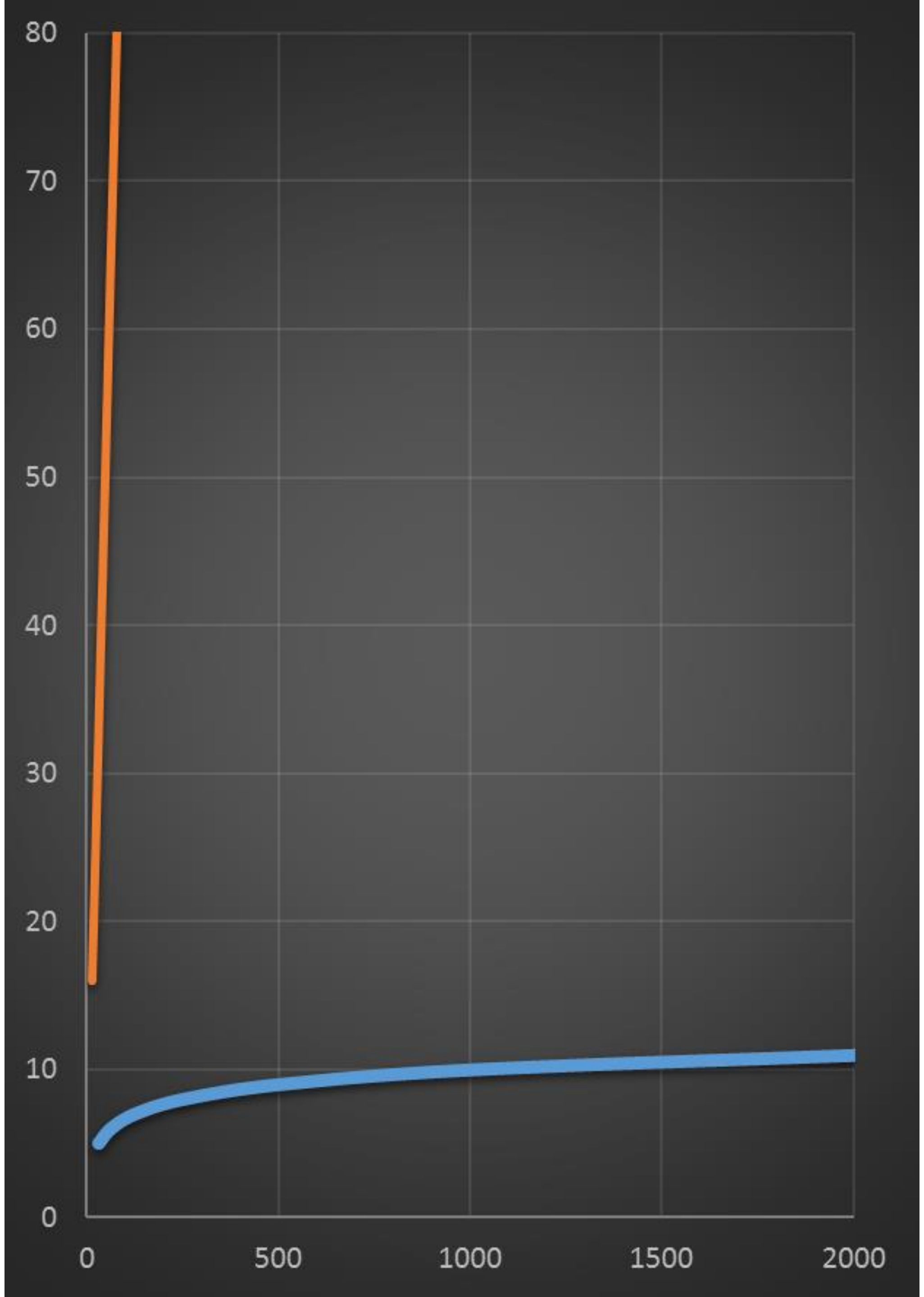
$$T(n) \in \mathcal{O}\left(f(n)\right) \text{ iff } \exists N \geq 0, c > 0,$$
$$T(n) \leq cf(n) \; \forall n \geq N$$

$$T(n) \in \Omega\left(f(n)\right) \text{ iff } \exists N \geq 0, l > 0,$$
$$T(n) \geq lf(n) \; \forall n \geq N$$

$$T(n) \in \Theta\left(f(n)\right) \text{ iff } \exists N \geq 0, c > 0, l > 0$$
$$lf(n) \leq T(n) \leq cf(n) \; \forall n \geq N$$

Complexity of the dictionary problem?

- How many comparisons as number of pages increases?
- Obviously less than linear growth…



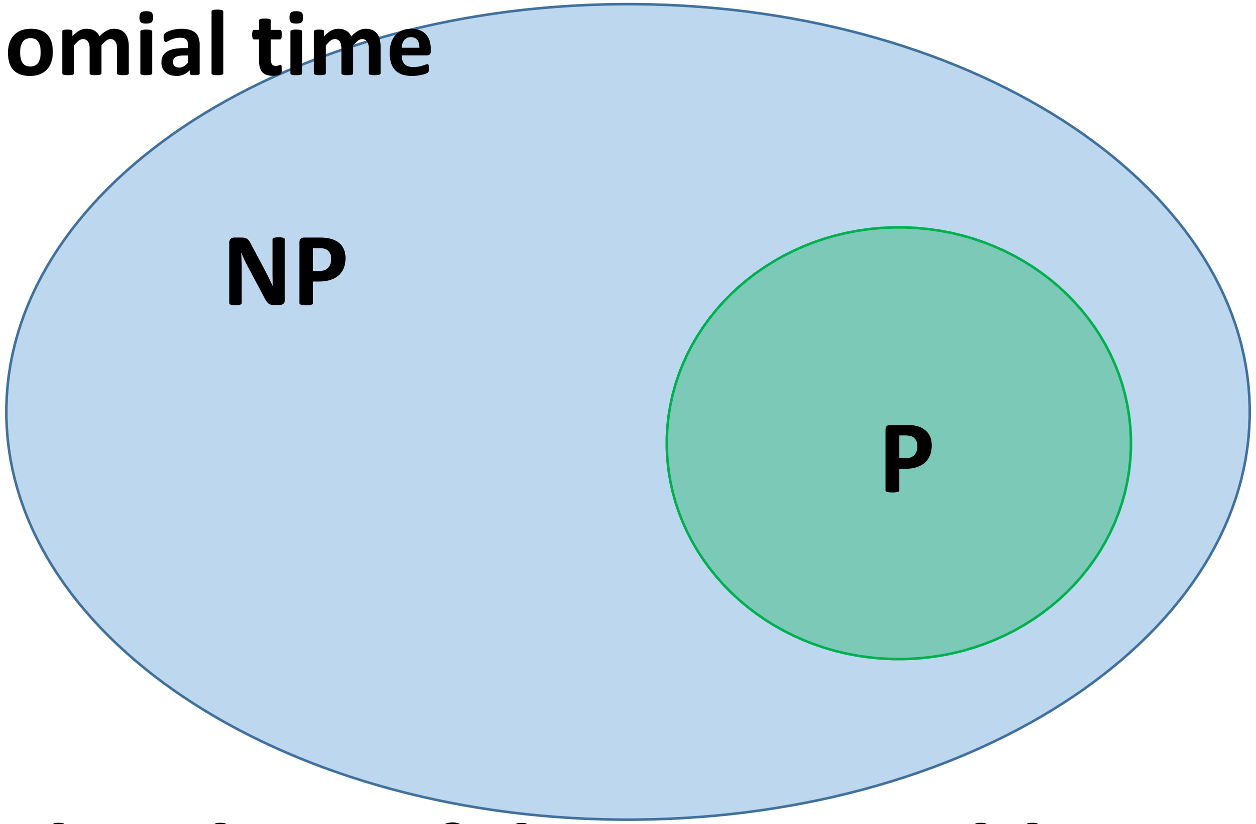
tractability

$\mathcal{O}(1)$	constant
$\mathcal{O}(\log n)$	logarithmic
$\mathcal{O}(n)$	linear
$\mathcal{O}(n \log n)$	loglinear
$\mathcal{O}(n^2)$	quadratic
$\mathcal{O}(n^c), c > 1$	polynomial
$\mathcal{O}(c^n)$	exponential
$\mathcal{O}(n!)$	factorial

Algorithms and complexity (VI)

P and NP (polynomial time and nondeterministic polynomial time)

NP: class of decision problems whose solutions can be <u>**verified**</u> in polynomial time



P: the class of decision problems that can be <u>**solved**</u> in polynomial time

decision problems vs. optimization problems

A decision problem asks us to check if something is true (possible answers: ‘yes’ or ‘no’)

e.g.,

PRIMES

Given: a positive integer ***n***

Question: is ***n*** prime?

decision problems vs. optimization problems

An optimization problem asks us to find, among all feasible solutions, one that maximizes or minimizes a given objective

e.g.,

SHORTEST PATH

Given: weighted graph G and two nodes ***s*** and ***t***

Problem: find shortest path from ***s*** to ***t***

KNAPSACK PROBLEM

Given: set of items and their value and volume, volume of knapsack

Problem: determine which items to select to maximize value

decision problems vs. optimization problems

A *decision version* of a given optimization problem can easily be defined using a bound on the value of feasible solutions

e.g.,

SHORTEST PATH DECISION PROBLEM

Given: weighted graph G and two nodes ***s*** and ***t***

Question: is there a path from ***s*** to ***t*** of length at most ***L?***

KNAPSACK DECISION PROBLEM

Given: set of items and their value and volume, volume of knapsack

Question: is there a combination of items that fit within the knapsack of value greater than or equal to ***V***?

discovery vs. verification

- Two important tasks for a scientist are discovery of solutions, and verification of other people’s solutions
- It is easier to check that a solution, say to a puzzle, is correct, rather than to find the solution
- That is, *verifying* a solution is easier than *discovering* it
- Example: Sudoku

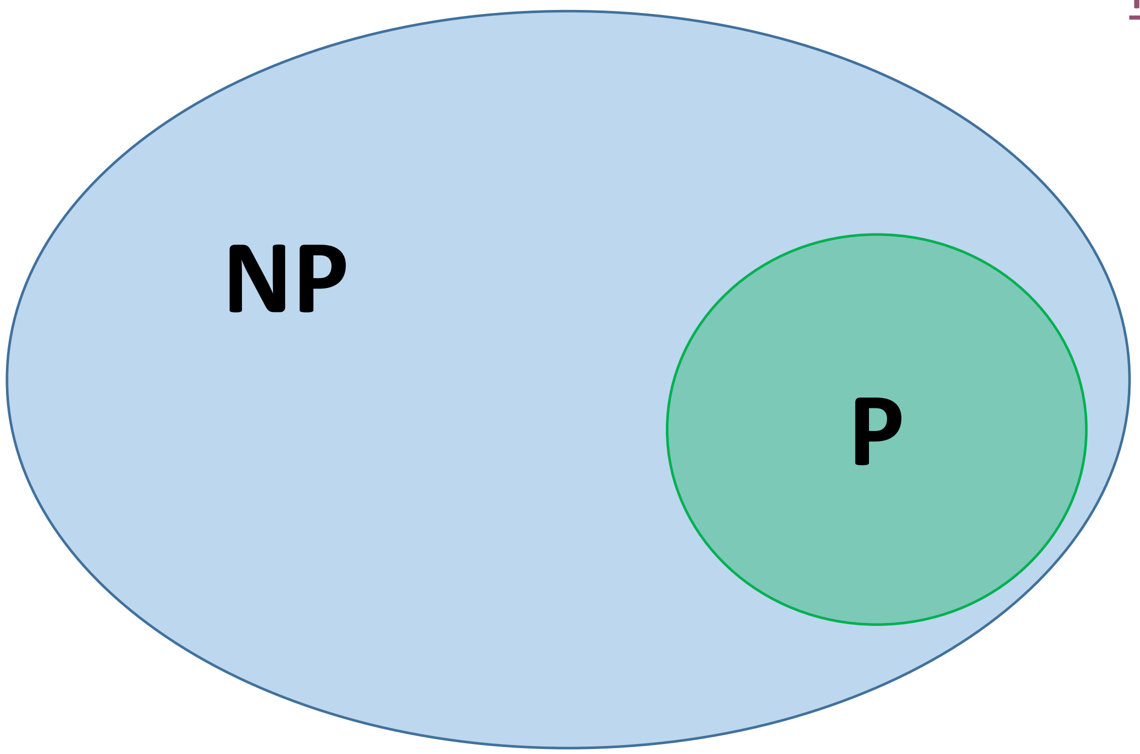
sudoku

9					1		5	
7	6	5						
1			3					8
					6		4	
			2	1	8			
	9		4					
6					4			2
						8	3	7
	3		1					5

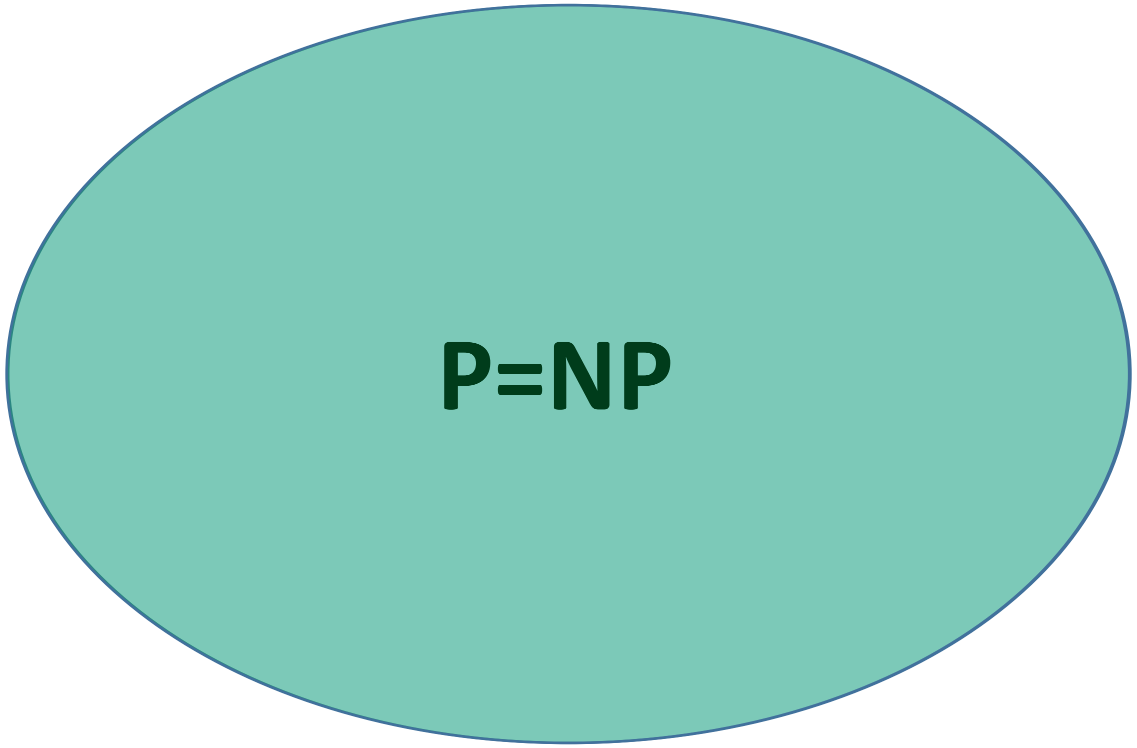
sudoku

9	8	3	7	2	1	6	5	4
7	6	5	8	4	9	3	2	1
1	2	4	3	6	5	7	9	8
8	1	7	9	5	6	2	4	3
3	4	6	2	1	8	5	7	9
5	9	2	4	7	3	1	8	6
6	7	8	5	3	4	9	1	2
4	5	1	6	9	2	8	3	7
2	3	9	1	8	7	4	6	5

http://www.claymath.org/millennium-problems

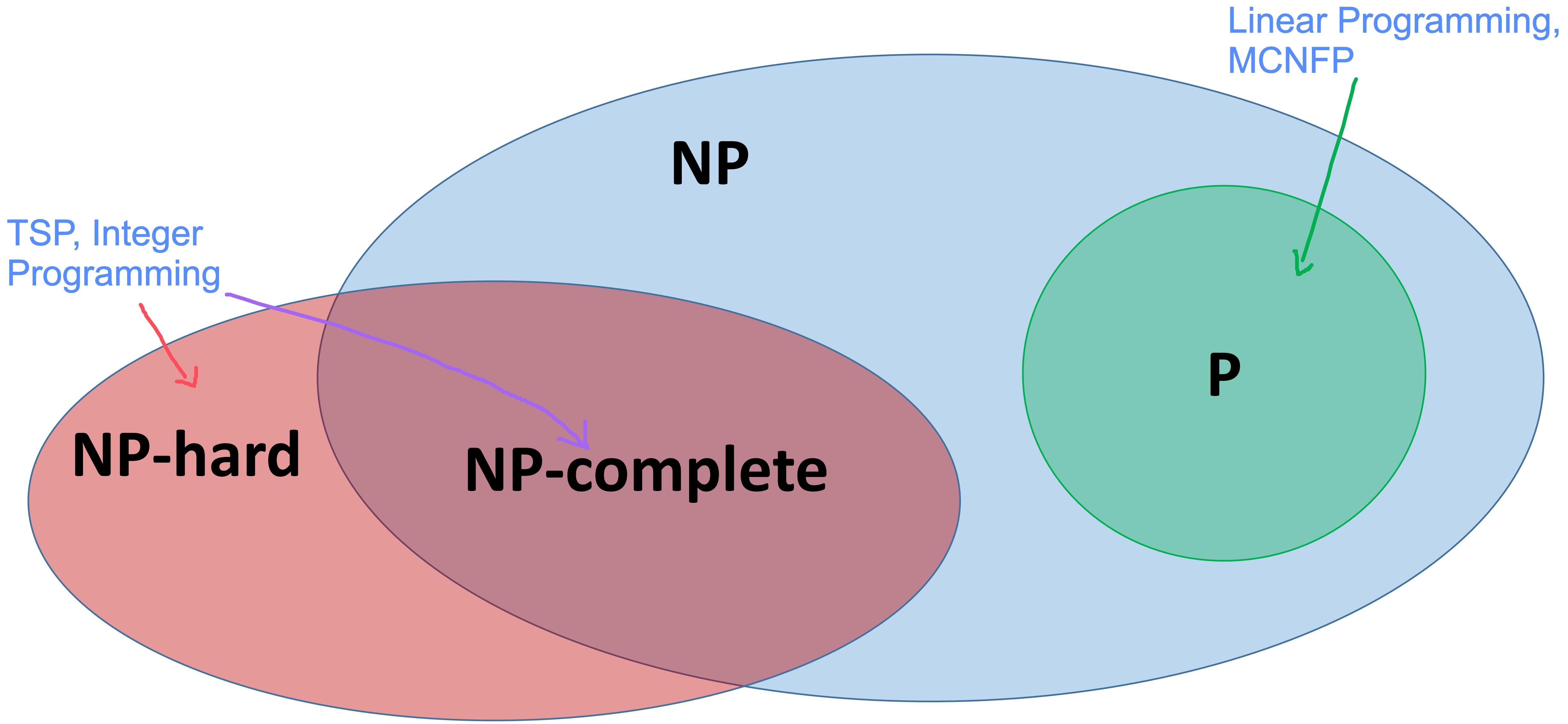


$$\mathbf{P} \subseteq \mathbf{NP}$$



$$\mathbf{P} = \mathbf{NP}?$$

The P vs. NP problem has been called “one of the deepest questions ever asked by human beings”


Linear Programming,
MCNFP
NP
TSP, Integer
Programming
P
NP-hard
NP-complete

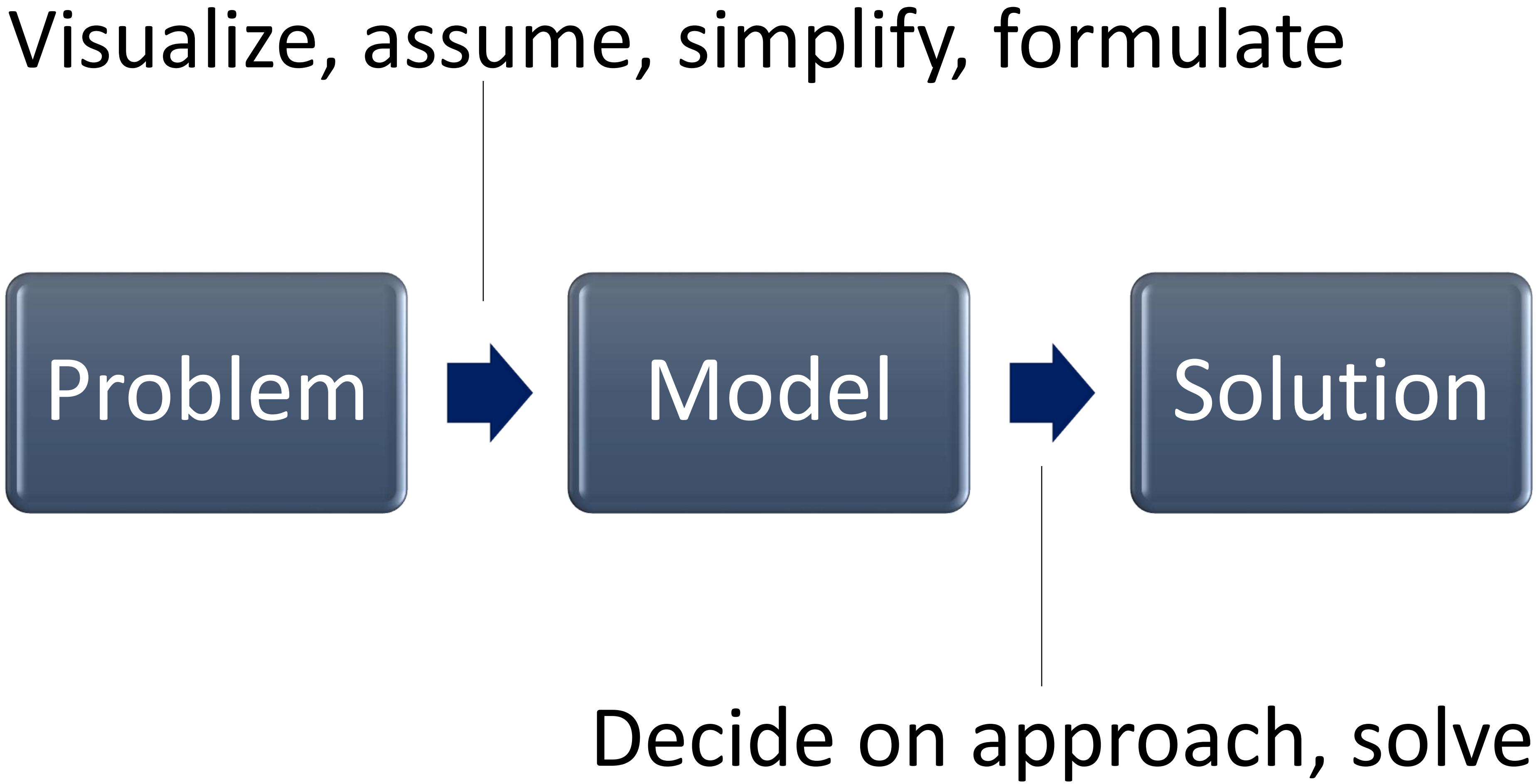
NP-complete problems are the "hardest" problems in NP

- Examples: Sudoku and 3-colorability

If there is a fast (polynomial-time) algorithm for *one* NP-complete problem, then there is a fast algorithm for *every* problem in NP!

- For example, a fast algorithm for Sudoku implies P=NP.

The decision versions of Integer programming, TSP, set-covering are all NP-complete. The optimization versions of the problems are NP-hard.


Visualize, assume, simplify, formulate
Problem
Model
Solution
Decide on approach, solve