Algorithms for Computational Biology

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$\boxed{\text{Computational efficiency II}}$

Computational efficiency of an algorithm is measured in terms of running time and storage space.

To abstract from

- specific computers (processor speed, computer architecture, ...)
- specific programming languages
- ...

we measure

- running time in number of (basic) operations
  (e.g. additions, multiplications, comparisons, ...),
- storage space in number of storage units
  (e.g. 1 unit = 1 integer, 1 character, 1 byte, ...).

Example DP algorithm for global alignment (Needleman-Wunsch), variant which outputs only $sim(s, t)$.

Algorithm *DP algorithm for global alignment*
Input: strings s, t, with $|s| = n, |t| = m$; scoring function (p, g)
Output: value $sim(s, t)$

1. **for** $j = 0$ to m **do** $D(0, j) \leftarrow j \cdot g$;
2. **for** $i = 1$ to n **do** $D(i, 0) \leftarrow i \cdot g$;
3. **for** $i = 1$ to n **do**
4. **for** $j = 1$ to m **do**
5. $$D(i,j) \leftarrow \max \begin{cases} D(i-1,j)+g \\ D(i-1,j-1)+p(s_i,t_j) \\ D(i,j-1)+g \end{cases}$$
6. **return** $D(n, m)$;

Analysis of DP algorithm for global alignment:

Time

- for first row: $m + 1$ operations (line 1)
- for first column: n operations (line 2)
- for each entry $D(i, j)$, where $1 \leq i \leq n, 1 \leq j \leq m$: 3 operations; there are $n \cdot m$ such entries: $3nm$ operations (lines 3-5)
- Altogether: $3nm + n + m + 1$ operations

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Equal length strings

If $n = m$ then time $= 3n^2 + 2n + 1$, space $= n^2 + 2n + 1$

Let's compare this with the other algorithm we saw for global alignment:

Exhaustive search

1. consider every possible alignment of s and t
2. for each of these, compute its score
3. output the maximum of these

Algorithm *Exhaustive search for global alignment*
Input: strings s, t, with $|s| = n, |t| = m$; scoring function (p, g)
Output: value $sim(s, t)$

1. int $max = (n + m)g$;
2. **for** each alignment A of s and t (in some order)
3. **do if** $score(A) > max$
4. **then** $max \leftarrow score(A)$;
5. **return** max;

Note:

1. The variable max is needed for storing the highest score so far seen.
2. The initial value of max is the score of *some* alignment of s, t (which one?)

Analysis of Exhaustive search:

Space

- Store one alignment at a time (overwrite with next one)

  Recall: if $\mathcal{A}$ al. of two strings of length n and m, then

  $$\max(n, m) \leq |\mathcal{A}| \leq (n + m).$$

  $\leq 2(n + m)$ units of storage (in each fits one integer or character)
  (2 bec. there are two rows)

- one storage unit for the variable *max*, the maximum seen so far: 1 unit of storage
- Equal length strings: space $\leq 4n$ units of storage

Analysis of Exhaustive search:

Time

- for every alignment (line 2.)
- compute its score (line 3.)

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For any al. $\mathcal{A}$, we have $\max(n, m) \leq |\mathcal{A}| \leq (n+m)$, *thus:*

$$N(n, m) \cdot \max(n, m) \leq \text{no. of steps} \leq N(n, m) \cdot (n+m)$$

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Simplify analysis: Let's look at two equal length strings $|s| = |t| = n$:

$$N(n, n) \cdot n \leq \text{no. of steps} \leq N(n, n) \cdot 2n$$

We have seen: $N(n, n) > 2^n$, so no. of steps $\geq 2^n \cdot n$.

Time comparison of the two algorithms

So we have, for $|s| = |t| = n$:

- DP algo: $3n^2 + 2n + 1$ operations
- Exhaustive search: at least $N(n, n) \cdot n$ operations

Let's compare the two functions for increasing n:

n	1	2	3	4	5	...	10	100	1000
$3n^2 + 2n + 1$	6	17	34	57	86	...	321	30 201	3 002 001
$N(n, n) \cdot n$	3	26	189	1284	8415	...	$\approx 80 \cdot 10^6$	$\approx 2 \cdot 10^{77}$	$\approx 10^{700}$

The DP algorithm is much faster than the exhaustive search algorithm, because its running time increases much slower as the input size increases. But how much?

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- We are interested in the algorithm's behaviour for large inputs.
- We want to know the growth behaviour, i.e. how time/space requirements change as input increases.
- We want an upper bound, i.e. on any input how much time/space needed at most? (worst-case analysis)

Consider 3 algorithms $\mathcal{A}, \mathcal{B}, \mathcal{C}$:

		input size n		
	running t.	10	20	What happened when input doubled?
$\mathcal{A}$	n	10		
$\mathcal{B}$	n^2	100		
$\mathcal{C}$	2^n	1024		

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Now 3 algorithms $\mathcal{A}', \mathcal{B}', \mathcal{C}'$:

		input size n		
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$\mathcal{A}'$	$3n$	30	60	
$\mathcal{B}'$	$3n^2$	300	1200	
$\mathcal{C}'$	$3 \cdot 2^n$	3072	3 145 728	

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The O-notation allows us to abstract from constants ($3n$ vs. n) and other details which are not important for the growth behaviour of functions.

Definition (O-classes)

Given a function $f : \mathbb{N} \to \mathbb{R}$, then $O(f(n))$ is the class (set) of functions $g(n)$ s.t.:

There exists a $c > 0$ and an $n_0 \in \mathbb{N}$ s.t. for all $n \geq n_0$: $g(n) \leq c \cdot f(n)$.

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Meaning: "g is smaller or equal than f (w.r.t. growth behaviour)"
"g does not grow faster than f"

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Proof

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Proof

Choose $c = 4$ and $n_0 = 3$. We have: $\forall n \geq 3 : \quad 3n^2 + 2n + 1 \leq 4n^2$.

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$$\begin{aligned} & 3n^2 + 2n + 1 \leq 4n^2 \\ \Leftrightarrow\quad & n^2 - 2n - 1 \geq 0 \\ \Leftrightarrow\quad & (n-1)^2 - 2 \geq 0 \\ \Leftrightarrow\quad & (n-1)^2 \geq 2 \\ \Leftrightarrow\quad & n \geq 3 \end{aligned}$$

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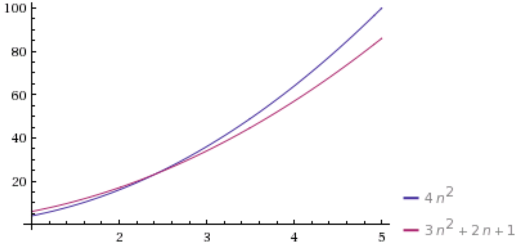

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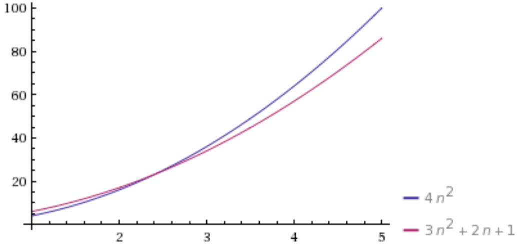
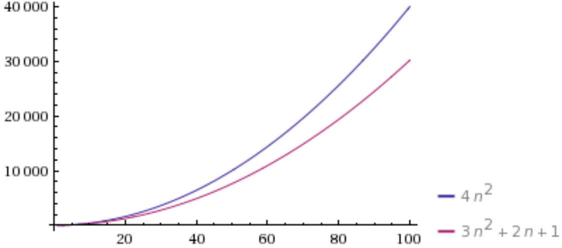
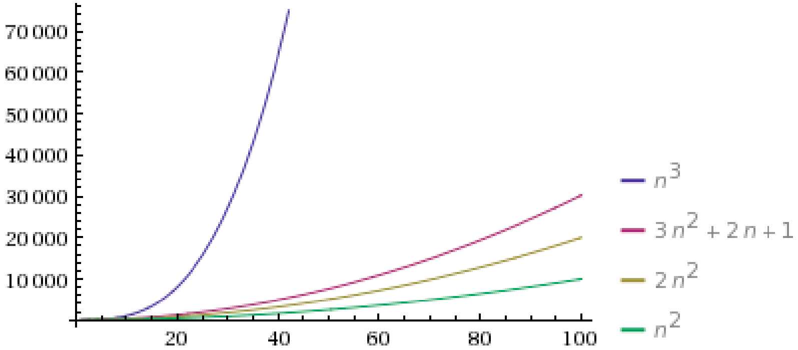




plot: WolframAlpha



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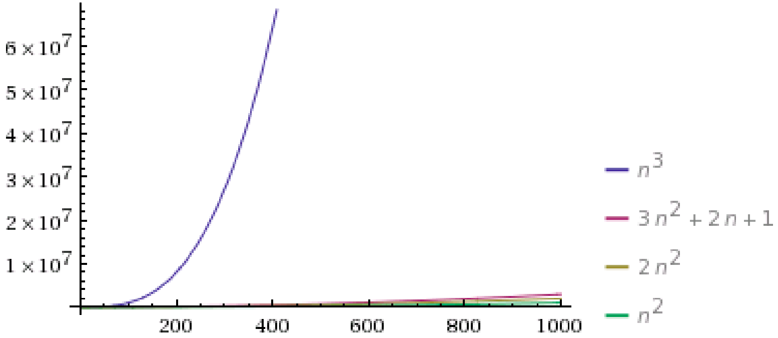

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In practice:

- identify which input parameters are important: no. months n for Fibonacci numbers; length of strings n, m for pairwise al.
- order additive terms according to these in decreasing growth order:
  $3n^5 + 2n^3 + n + 7$,
  $3nm + n + m + 1$
- take largest without multiplicative constant:
  $3n^5 + 2n^3 + n + 7 \in O(n^5)$,
  $3nm + n + m + 1 \in O(nm)$

Important O-classes

The most important functions, ordered by increasing O–classes: each function f_i is in the O–class of the next function f_{i+1}, but $f_{i+1}(n) \notin O(f_i(n))$.

1	$\log \log n$	$\log n$	$\sqrt{n}$	n	$n \log n$	n^2	n^3	$\dots$	$\dots$	2^n	$n!$	n^n
constant		logarithmic		linear		quadratic	cubic			exponential		
			polynomial (of the form n^c for some constant c) (all except $n \log n$ are polynomials)									
E F F I C I E N T[1]									inefficient			

function grows slower $\longleftrightarrow$ *function grows faster*

faster algorithm — *slower algorithm*

[1]also called *feasible* vs. *infeasible*

Amount of time an algorithm of time complexity $f(n)$ would need on a computer that performs one million operations per second:

$f(n)$	$n = 50$	$n = 100$	$n = 200$
n	$5 \cdot 10^{-5}$ s	10^{-4} s	
n^2	0.0025 s	0.01 s	
n^3	0.125 s	1 s	
1.1^n	0.0001 s	0.014 s	
2^n	35.7 years	$4 \cdot 10^{16}$ years	

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Age of the universe $\approx 4.3 \cdot 10^{17}$ s $\approx 1.4 \cdot 10^{10}$ years
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n^3	0.125 s	1 s	8 s
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2^n	35.7 years	$4 \cdot 10^{16}$ years	$5 \cdot 10^{46}$ years

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On a 1000 times faster computer:

$f(n)$	$n = 50$	$n = 100$	$n = 200$
n	$5 \cdot 10^{-8}$ s	10^{-7} s	$2 \cdot 10^{-7}$ s
n^2	$2.5 \cdot 10^{-6}$ s	10^{-5} s	$4 \cdot 10^{-5}$ s
n^3	$1.25 \cdot 10^{-4}$ s	10^{-3} s	$8 \cdot 10^{-3}$ s
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Looking at it in a different way ...

	1	2	3	4	5	...	10	20	100	1000	10^6
n	1	2	3	4	5	...	10	20	100	1000	10^6
n^2	1	4	9	16	25	...	100	400	10000	10^6	
2^n	2	4	8	16	32	...	1024	$\approx 10^6$	$\approx 10^{30}$	$\approx 10^{301}$	

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On a computer that can perform one million operations per second, in a second,

- a linear-time algorithm can solve a problem instance of size 10^6 (one million) (e.g. fib2, fib3),
- a quadratic-time algorithm one of size 1000 (one thousand),
- an exponential-time algorithm one of size 20 (e.g. fib1).

In fact, on any computer, these algorithms need always the same amount of time for problem instances of such different sizes!

Back to the global alignment algorithms:

- $A(n) := 3n^2 + 2n + 1$ running time of DP algo
- $B(n) := n \cdot N(n, n)$ running time of exhaustive search algo

	1	2	3	4	5	...	10	20	100	1000
$A(n)$	6	17	34	57	86	...	321	1241	30 201	3 002 001
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- $A(n) \in O(n^2)$ a quadratic time algorithm
- $B(n)$ is super-exponential time

Age of the universe $\approx 4.3 \cdot 10^{17}$ s $\approx 1.4 \cdot 10^{10}$ years

e.g. $5 \cdot 10^{16}$ op's $= 5 \cdot 10^7 s \approx 575$ days, if we have 1 billion (10^9) ops/s