Algorithms for Computational Biology

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Computational efficiency I



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Computational Efficiency

As we will see later in more detail, the efficiency of algorithms is measured w.r.t.

- running time: how long does it take?
- storage space: how much memory in the computer does it occupy?

We will make these concepts more concrete later on, but for now want to give some intuition, using an example.

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Example: Computation of nth Fibonacci number

Leonardo Fibonacci (1170 - 1240) a.k.a. Leonardo of Pisa

Fibonacci numbers: model for growth of populations (simplified model)

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Example: Computation of *n*th Fibonacci number

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• Start with 1 pair of rabbits in the field

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- Start with 1 pair of rabbits in the field
- each pair becomes mature at age of 1 month and mates

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 $^{^{1}}$ This unrealistic assumption simplifies the mathematics; however, it turns out that adding a certain age at which rabbits die does not significantly change the behaviour of the sequence, so it makes sense to simplify.

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- after gestation period of 1 month, a female gives birth to 1 new pair
- rabbits never die¹

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- after gestation period of 1 month, a female gives birth to 1 new pair
- rabbits never die1

Definition

F(n) = number of pairs of rabbits in field at the beginning of the *n*th month

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The nth Fibonacci number

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month 1:

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• month 1: there is 1 pair of rabbits in the field F(1) = 1

• month 2:

The *n*th Fibonacci number

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• month 1: there is 1 pair of rabbits in the field

F(1) = 1

• month 2: there is still 1 pair of rabbits in the field

F(2) = 1

• month 3:

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F(1) = 1

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• month 1: there is 1 pair of rabbits in the field

• month 2: there is still 1 pair of rabbits in the field F(2) = 1

• month 3: there is the old pair and 1 new pair F(3) = 1 + 1 = 2

• month 4:

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• month 1: there is 1 pair of rabbits in the field

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F(2) = 1

month 3: there is the old pair and 1 new pair

F(3) = 1 + 1 = 2

• month 4: the 2 pairs from previous month, plus the old pair has had another new pair

F(4) = 2 + 1 = 3

• month 5:

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• month 1: there is 1 pair of rabbits in the field

F(1) = 1

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• month 2: there is still 1 pair of rabbits in the field

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F(4) = 2 + 1 = 3

• month 5: the 3 from previous month, plus

the 2 from month 3 have each had a new pair

F(5) = 3 + 2 = 5

The nth Fibonacci number

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• month 1: there is 1 pair of rabbits in the field

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• month 2: there is still 1 pair of rabbits in the field

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F(4) = 2 + 1 = 3

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Recursion for Fibonacci numbers

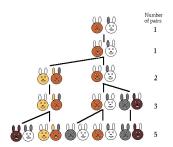
$$F(1) = F(2) = 1$$

for $n > 2$: $F(n) = F(n-1) + F(n-2)$.

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The nth Fibonacci number



 ${\color{red} \textbf{source:}} \ \, \textbf{Fibonacci numbers and nature} \\ (\text{http://www.maths.surrey.ac.uk/hosted-sites/R.Knott/Fibonacci/fibnat.html}) \\$

The nth Fibonacci number

The first few terms of the Fibonacci sequence are:

 n
 1
 2
 3
 4
 5
 6
 7
 8
 9
 10
 11
 12

 n)
 1
 1
 2
 3
 5
 8
 13
 21
 34
 55
 89
 144
 13 233

The *n*th Fibonacci number

The first few terms of the Fibonacci sequence are:

n	1	2	3	4	5	6	7	8	9	10	11	12	13	14	
F(n)	1	1	2	3	5	8	13	21	34	55	89	144	233	377	-
. ,															
n	1	5	16		17		18	1	19	20		21	22		23
$\overline{F(n)}$	61	0	987	1	597	2	584	4 18	31	6 765	10	946	17 711	28	557

Fibonacci numbers in nature



source: Plant Spiral Exhibit
(http://cs.smith.edu/ phyllo/Assets/Images/ExpoImages/ExpoTour/index.htm)
On these pages it is explained how these plants develop. Very interesting!

Fibonacci numbers in nature

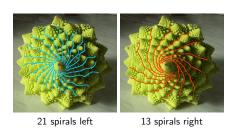


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Fibonacci numbers in nature



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very nice page! recommended!

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Growth of Fibonacci numbers

Theorem

For $n \ge 6$: $F(n) > (1.5)^{n-1}$.

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For $n \ge 6$: $F(n) > (1.5)^{n-1}$.

n	1	2	3	4	5	6	7
F(n)	1	1	2	3	5	8	13
$(3/2)^{n-1}$							

Growth of Fibonacci numbers

Theorem

For $n \ge 6$: $F(n) > (1.5)^{n-1}$.

n	1	2	3	4	5	6	7
<i>F</i> (<i>n</i>)	1	1	2	3	5	8	13
$(3/2)^{n-1}$	1	1.5	2.25	3.375	\sim 5.06	\sim 7.59	~ 11.39

n	8	9	10	11	12	13	14
F(n)	21	34				233	377
$(3/2)^{n-1}$	$\sim \! 17.09$	\sim 25.63					\sim 194.62

 \sim : rounded to two decimals

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Growth of Fibonacci numbers

Theorem

For $n \ge 6$: $F(n) > (1.5)^{n-1}$.

Growth of Fibonacci numbers

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For $n \ge 6$: $F(n) > (1.5)^{n-1}$.

Proof

Note that from n=3 on, F(n) strictly increases, so for $n\geq 4$, we have F(n-1)>F(n-2). Therefore, $F(n-1)>\frac{1}{2}F(n)$, since F(n)=F(n-1)+F(n-2).

We prove the theorem by induction:

Base: For n = 6, we have $F(6) = 8 > 7.59375 = (1.5)^5$.

Step: Now we want to show that $F(n+1)>(1.5)^n$. By the I.H. (induction hypothesis), we have that $F(n)>(1.5)^{n-1}$. Since F(n-1)>0.5F(n), it follows that $F(n+1)=F(n)+F(n-1)>1.5\cdot F(n)>(1.5)\cdot (1.5)^{n-1}=(1.5)^n$.

Growth of Fibonacci numbers

Theorem

For $n \ge 6$: $F(n) > (1.5)^{n-1}$.

Question:

Why is this interesting?

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Growth of Fibonacci numbers

Theorem

For $n \ge 6$: $F(n) > (1.5)^{n-1}$.

Question:

Why is this interesting?

Answer

Because it means that the Fibonacci numbers increase exponentially.

- 1.5^{n-1} has exponential growth (in n)
- base: 1.5 (greater than 1)
- exponent: n-1

We will come back to this later.

Computation of nth Fibonacci number

Def:
$$F(1) = F(2) = 1$$
, and $n > 2$: $F(n) = F(n-1) + F(n-2)$.

Algorithm 1 (let's call it $\mbox{fib1}$) works exactly along the recursive definition:

Algorithm fib1(n)

- 1. **if** n = 1 or n = 2
- 2. then return 1
- else
- 4. **return** fib1(n-1) + fib1(n-2)

Computation of nth Fibonacci number

Analysis

(sketch) Looking at the computation tree, we can see that the tree for computing F(n) has F(n) many leaves (show by induction), where we have a lookup for F(2) or F(1). A binary rooted tree has one fewer internal nodes than leaves (see second part of course, or show by induction), so this tree has F(n) - 1 internal nodes, each of which entails an addition. So for computing F(n), we need F(n) lookups and F(n)-1additions, altogether 2F(n) - 1 operations (additions, lookups etc.).

The algorithm has exponential running time, since it makes 2F(n)-1, i.e. at least $2\cdot (1.5)^{n-1}-1$ steps (operations).

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Computation of nth Fibonacci number

Algorithm 3 (let's call it fib3) computes F(n) iteratively, like Algorithm 2, but using only 3 units of storage space.

Algorithm fib3(n)

return c;

```
int a, b, c;
2
       a \leftarrow 1; b \leftarrow 1; c \leftarrow 1;
3.
       for k = 3 \dots n
4.
             do c \leftarrow a + b;
5.
                  a \leftarrow b; b \leftarrow c;
6.
```

Analysis

(sketch) Time: same as Algo 2. Uses 3 units of storage (called a, b, and c).—The algorithm has linear running time and constant storage space.

Summary

- We saw 3 different algorithms for the same problem (computing the nth Fibonacci number).
- They differ greatly in their efficiency:
 - Algo fib1 has exponential running time.
 - Algo fib2 has linear running time and linear storage space.
 - Algo fib3 has linear running time and constant storage space.
- We saw on an example computation (during class) that exponential running time is not practicable.

Computation of nth Fibonacci number

Algorithm 2 (let's call it fib2) computes every F(k), for $k = 1 \dots n$, iteratively (one after another), until we get to F(n).

Algorithm fib2(n)

```
array of int F[1 \dots n];
1.
      F[1] \leftarrow 1; F[2] \leftarrow 1;
      for k = 3...n
do F[k] \leftarrow F[k-1] + F[k-2];
3.
4.
       return F[n];
```

Analysis

(sketch) One addition for every $k=1,\ldots,n$. Uses an array of integers of length n.—The algorithm has linear running time and linear storage space.

Comparison of running times

	n	1	2	3	4	5	6	7	10	20	30	40
-	F(n)	1	1	2	3	5	8	13	55	6 765	832 040	102 334 155
	fib1	1	1	3	5	9	15	25	109	13 529	1 664 079	204 668 309
	fib2	1	2	3	4	5	6	7		20	30	40
	fib3	1	2	3	4	5	6	7	10	20	30	40

The number of steps each algorithm makes to compute F(n).

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Summary (2)

Take-home message

- There may be more than one way of computing something.
- It is very important to use efficient algorithms.
- Efficiency is measured in terms of running time and storage space.
- Computation time is important for obvious reasons: the faster the algorithm, the more problems we can solve in the same amount of
- In computational biology, inputs are often very large, therefore storage space is at least as important as running time: if you run out of storage space, you cannot complete the computation.

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