Algorithms for Computational Biology

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Computational efficiency I


FoxTrot
by Bill Amend
ONE CHEESY TORTILLA CHIP...
ONE CHEESY TORTILLA CHIP...
TWO CHEESY TORTILLA CHIPS...
THREE CHEESY TORTILLA CHIPS...
FIVE CHEESY TORTILLA CHIPS...
EIGHT CHEESY TORTILLA CHIPS...
MATH GEEKS SHOULDN'T BE ALLOWED ANYWHERE NEAR CERTAIN FOODS.
WHAT'S WRONG WITH FIBONACHOS?
THERE'RE ONLY 12 LEFT...NOW WHAT?
www.foxtrot.com

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.

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)

[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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Definition

$F(n) =$ number of pairs of rabbits in field at the beginning of the nth month.

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The nth Fibonacci number

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- month 1:

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- month 2:

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- month 3:

The nth Fibonacci number

$F(n) =$ number of pages of rabbits in field

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- month 3: there is the old pair and 1 new pair $F(3) = 1 + 1 = 2$
- month 4:

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- 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 4: the 2 pairs from previous month, plus the old pair has had another new pair $F(4) = 2 + 1 = 3$
- month 5: the 3 from previous month, plus the 2 from month 3 have each had a new pair $F(5) = 3 + 2 = 5$

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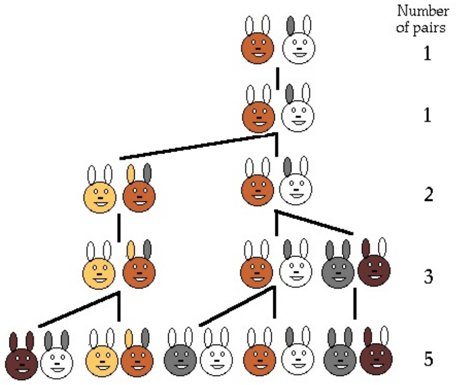
Recursion for Fibonacci numbers

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

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

The *n*th Fibonacci number



source: Fibonacci numbers and nature
(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	13	14
$F(n)$	1	1	2	3	5	8	13	21	34	55	89	144	233	377

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n	15	16	17	18	19	20	21	22	23
$F(n)$	610	987	1 597	2 584	4 181	6 765	10 946	17 711	28 657

Fibonacci numbers in nature

21 spirals left

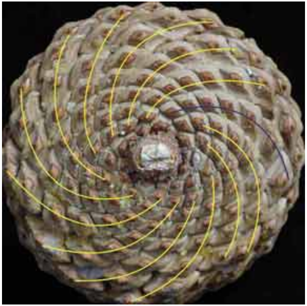
34 spirals right

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

8 spirals left



13 spirals right

source: Plant Spiral Exhibit
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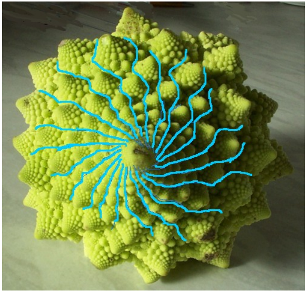

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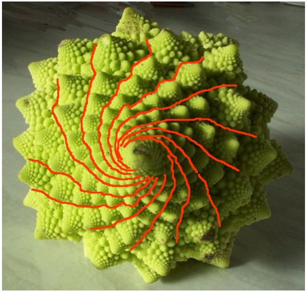

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very nice page! recommended!

Growth of Fibonacci numbers

Theorem

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

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

Growth of Fibonacci numbers

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

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

n	8	9	10	11	12	13	14
$F(n)$	21	34	55	89	144	233	377
$(3/2)^{n-1}$	$\sim$17.09	$\sim$25.63	...	...	...	...	$\sim$194.62

$\sim$: rounded to two decimals

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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

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Question:

Why is this interesting?

Growth of Fibonacci numbers

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

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 *n*th 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 fib1) works exactly along the recursive definition:

Algorithm *fib1(n)*

```
if n = 1 or n = 2
    then return 1
    else
        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 $F(n) - 1$ additions, 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).

Computation of nth Fibonacci number

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

Algorithm *fib2(n)*

```
array of int F[1...n];
F[1] ← 1; F[2] ← 1;
for k = 3...n
    do F[k] ← F[k − 1] + F[k − 2];
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.

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)*

```
int a, b, c;
a ← 1; b ← 1; c ← 1;
for k = 3 ... n
    do c ← a + b;
       a ← b; b ← c;
return c;
```

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.

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	10	20	30	40
fib3	1	2	3	4	5	6	7	10	20	30	40

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

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.

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 time.
- 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.