Übungen zu Algorithmen und Programmentwicklung für die Biologische Chemie

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(based on slides by Sven Findeiß)

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Sommersemester 2021

Dynamic Progamming

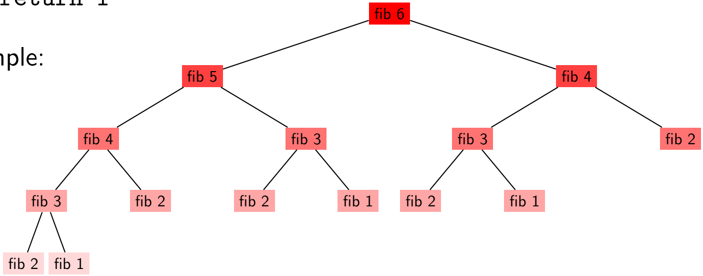
- Solving recursion equations (with overlapping subproblems) efficiently
- Optimization employing 'optimal substructure'

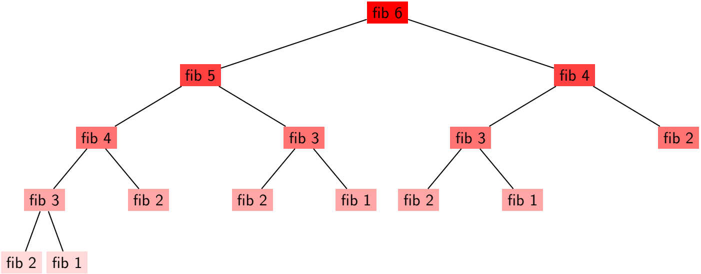
Example 1: Fibonacci Series

The Fibonacci Series of numbers 1, 1, 2, 3, 5, 8, 13, 21, 34, ... can be defined recursively:

```
def fib(n):
    if n <= 2:  f = 1
    else:       f = fib(n-1) + fib(n-2)
    return f
```

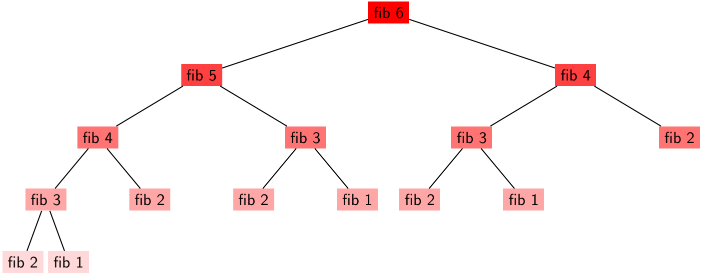
Example:





Building the solution space we realize:

1. The run-time of the recursion scales exponentially ($\sim 2^n$) with the input size.
2. Many (sub)solutions are calculated over and over again ($5 \times$ `fib 2`, $3 \times$ `fib 3`, $2 \times$ `fib 4`).
3. Avoid redundancy: tabulate subsolutions!



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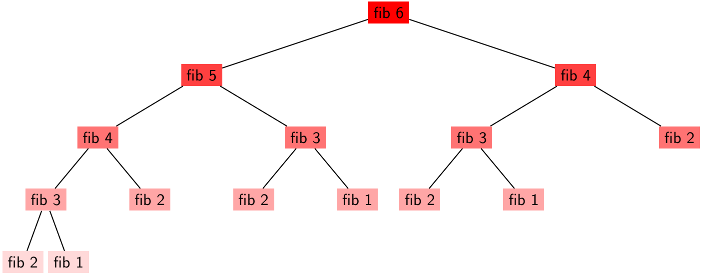

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memo = {}
def fib(n):
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        return memo[n]
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Stop and think:

- How much faster can one compute fib using DP?
- How much space do we need for DP-fib?

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def fib(n):

    for i in range(1,n+1):
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        else:
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        memo[i] = f
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```

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Optimization by DP: Levenshtein Distance

Definition: *Levenshtein distance of strings a and b* := minimal cost of transforming *a* into *b* by edit operations "replace", "insert", "delete" each of cost 1.

Example: `AUTO` ⇒ `RAD`, `MOTORRAD` ⇒ `FAHRRAD`

As edit sequence:

`AUTO` → `AUT` → `AUD` → `AD` → `RAD` (4)

`MOTORRAD` → `MOTHRRAD` → `MOAHRRAD` → `MFAHRRAD` → `FAHRRAD` (4)

or as alignment:

```
-AUTO        MOTORRAD
RA-D-        -FAHRRAD
```

NOTE: "Levenshtein Distance" has *optimal substructure*:
If `-AUTO` / `RA-D-` is optimal, then it's subsolution `-AUT` / `RA-D` (of subproblem 'AUT' vs. 'RAD') must be optimal.

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Calculating the Levenshtein distance of a and b

- build $n \times m$-matrix D
  where: $D_{ij} :=$ distance of $a_1, \ldots, a_i$ and $b_1, \ldots, b_j$
- calculate each D_{ij} from optimal partial solutions

Recursion:

$$D_{0,0} = 0; D_{0,j} = j; D_{i,0} = i$$

$$D_{i,j} = min \begin{cases} D_{i-1,j-1} + \begin{cases} 1 & \text{if } a_i \neq b_j \\ 0 & \text{otherwise} \end{cases} \\ D_{i-1,j} + 1 \\ D_{i,j-1} + 1 \end{cases}$$

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	j	0	1	2	3
i		-	R	A	D
0	-	0	1	2	3
1	A	1			
2	U	2			
3	T	3			
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$D_{n,m}$ contains the distance of a and b.

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$D_{n,m}$ contains the distance of a and b.

Tracing back the optimal choices from $D_{n,m}$ to $D_{0,0}$ yields *some* optimum alignment of a and b.

Assignment A3: Optimization by DP

Go to:

`https://github.com/TBIAPBC/APBC2021/tree/master/A3`

Happy hacking!