Übungen zu Algorithmen und Programmentwicklung für die Biologische Chemie

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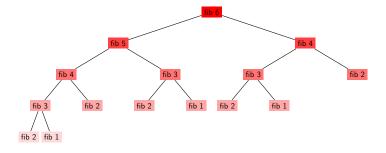
Dynamic Progamming

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

Example 1: Fibonacci Series

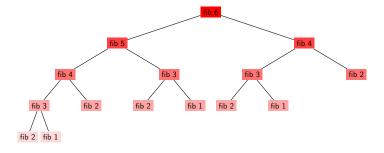
The Fibonacci Series of numbers 1, 1, 2, 3, 5, 8, 13, 21, 34, ... can be defined recursively:

```
def fib(n):
     if n \le 2: f = 1
     else: f = fib(n-1) + fib(n-2)
     return f
Example:
                                                                fib 2
       fib 3
                 fib 2
                                                  fib 1
                          fib 2
                                   fib 1
                                         fib 2
     fib 2 fib 1
```



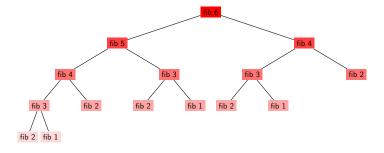
Building the solution space we realize:

- **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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```
memo = \{\}
                                   def fib(n):
def fib(n):
                                        if n in memo:
    if n \le 2:
                                            return memo[n]
        f = 1
                                        elif n \leq 2:
    else:
                                            f = 1
        f = fib(n-1)
                                        else:
             + fib(n-2)
                                            f = fib(n-1)
    return f
                                                + fib(n-2)
                                       memo[n] = f
                                        return f
```

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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Recursive (top-down) vs. iterative (bottom-up) Fibonacci

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memo = \{\}
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def fib(n):
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    if n in memo:
        return memo[n]
                                    for i in range(1,n+1):
    elif n \le 2:
                                        if i <= 2:
                                            f = 1
        f = 1
    else:
                                        else:
        f = fib(n-1)
                                            f = memo[i-1]
             + fib(n-2)
                                                 + memo[i-2]
                                        memo[i] = f
    memo[n] = f
    return f
                                    return memo[n]
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OP = Order + Tabulation (Reuse)

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                                        else:
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                                                 + memo[i-2]
                                        memo[i] = f
    memo[n] = f
    return f
                                    return memo[n]
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DP = Order + Tabulation (Reuse)

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 \Rightarrow RAD, MOTORRAD \Rightarrow FAHRRAD

As edit sequence:

$$\texttt{AUTO} \ \to \ \texttt{AUT} \ \to \ \texttt{AUD} \ \to \ \texttt{AD} \ \to \ \texttt{RAD} \tag{4}$$

$$ext{MOTORRAD}
ightarrow ext{MOTHRRAD}
ightarrow ext{MOAHRRAD}
ightarrow ext{MFAHRRAD}
ightarrow ext{FAHRRAD}$$

or as alignment: -AUTO MOTORRAD

RA-D- -FAHRRAD

NOTE: "Levenshtein Distance" has optimal substructure:

If -AUTO is optimal, then it's subsolution -AUT (of
RA-DRA-D
subproblem 'AUT' vs 'RAD') must be optimal

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Calculating the Levenshtein distance of a and b

- build n × m-matrix D
 where: D_{ij} := distance of a₁,..., a_i and b₁,..., b_j
- calculate each D_{ij} from optimal partial solutions

Recursion:

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

$$D_{i,j} = min \left\{ egin{array}{ll} D_{i-1,j-1} + egin{array}{ll} 1 & ext{if } a_i
eq b_j \ 0 & ext{otherwise} \ D_{i-1,j} + 1 \ D_{i,j-1} + 1 \end{array}
ight.$$

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

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

	j	0	1	2	3
i		-	R	Α	D
0	-	0	1	2	3
1	Α	1			
2	U	2			
2 3 4	T	3			
4	0	4			

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i		-	R	Α	D
0	-	0	1	2	3
1	Α	1	1	1	2
2	U	2	2	2	2
3	Т	3	3	3	3
4	0	4	4	4	4

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4	0	4			

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i		-	R	Α	D
0	-	0	1	2	3
1	Α	1	1	1	2
2	U	2	2	2	2
3	Т	3	3	3	3
4	0	4	4	4	4

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

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

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	j	0	1	2	3
i		-	R	Α	D
0	-	0	1	2	3
1	Α	1			
2	U	2			
3	T	3			
4	0	4			

j	0	1	2	3
	-	R	Α	D
-	0	1	2	3
Α	1	1	1	2
U	2	2	2	2
Т	3	3	3	3
0	4	4	4	4
	T	- 0 A 1 U 2 T 3	- R - 0 1 A 1 1 U 2 2 T 3 3	- R A - 0 1 2 A 1 1 1 U 2 2 2 T 3 3 3

 $D_{n,m}$ 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/APBC2025/tree/master/A3

Happy hacking!