Introduction to Optimization

Lecture 6: Discrete Optimization II

November 15, 2019

TC2 - Optimisation

Université Paris-Saclay

Anne Auger and Dimo Brockhoff

Inria Saclay – Ile-de-France

Course Overview

Date		Topic
Fri, 27.9.2019	DB	Introduction
Fri, 4.10.2019 (4hrs)	AA	Continuous Optimization I: differentiability, gradients, convexity, optimality conditions
Fri, 11.10.2019 (4hrs)	AA	Continuous Optimization II: constrained optimization, gradient-based algorithms, stochastic gradient
Fri, 18.10.2019 (4hrs)	DB	Continuous Optimization III: stochastic algorithms, derivative-free optimization, ~~critical performance assessment~~ [1st written test]
Wed, 30.10.2019	DB	Benchmarking + Discrete Optimization I: graph theory, greedy algorithms
Fri, 15.11.2019	DB	Discrete Optimization II: greedy algorithms II, dynamic programming, (heuristics) [2nd written test]
Fri, 22.11.2018		final exam

Back to Greedy Algorithms

Reminder: Greedy Algorithms

From Wikipedia:

> "A *greedy algorithm* is an algorithm that follows the problem solving *heuristic* of making the locally optimal choice at each stage with the hope of finding a global optimum."

- Note: typically greedy algorithms do not find the global optimum

Lecture Outline Greedy Algorithms

What we saw:

❶ Example 1: Money Change problem

What we will do today:

❷ Example 2: Minimal Spanning Trees (MST) and the algorithm of Kruskal

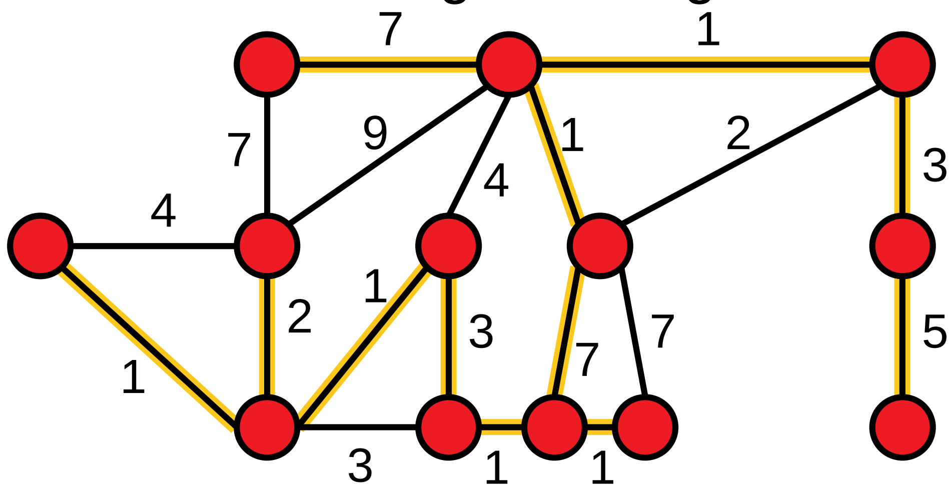
Example 2: Minimum Spanning Trees (MST)

Minimum Spanning Tree problem:

Given a graph G=(V,E) with edge weights w_i for each edge e_i. Find the spanning tree with the smallest weight among all spanning trees.

weight of a spanning tree:

$$w(T) = \sum_{e_i \text{ in } T} w_i$$



w(T) = 33

Applications

Setting up a new wired telecommunication/water supply/electricity network

Constructing minimal delay trees for broadcasting in networks

Kruskal's Algorithm: Idea

Algorithm, see [1]

- Create forest F = (V,{}) with n components and no edge
- Put sorted edges (such that w.l.o.g. $w_1 < w_2 < \ldots < w_{|E|}$) into set S
- While S non-empty and F not spanning:
  - delete cheapest edge from S
  - add it to F if no cycle is introduced

[1] Kruskal, J. B. (1956). "On the shortest spanning subtree of a graph and the traveling salesman problem". *Proceedings of the American Mathematical Society* **7**: 48–50. doi:10.1090/S0002-9939-1956-0078686-7

Kruskal's Algorithm: Runtime Considerations

First question: how to implement the algorithm?

- sorting of edges needs O(|E| log |E|)

Algorithm

```
Create forest F = (V,{}) with n components and no edge
Put sorted edges (such that w.l.o.g. $w_1 < w_2 < ... < w_{|E|}$) into set S
While S non-empty and F not spanning:
        delete cheapest edge from S
        add it to F if no cycle is introduced
```

simple

?

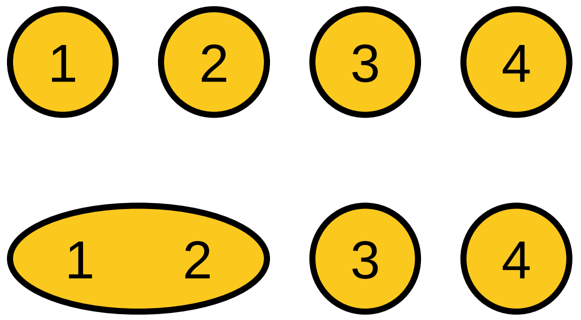
forest implementation:
Disjoint-set data structure

Disjoint-set Data Structure ("Union&Find")

Data structure: ground set 1...N grouped to disjoint sets

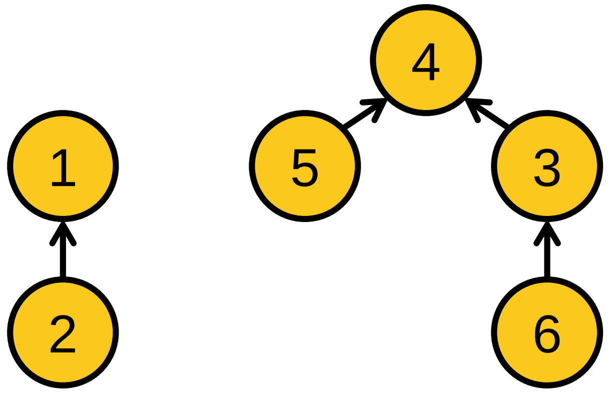
Operations:

- FIND(i): to which set does i belong?
- UNION(i,j): union the sets of i and j!



Implemented as trees:

- UNION(T1, T2): hang root node of smaller tree under root node of larger tree (constant time), thus
- FIND(u): traverse tree from u to root (to return a representative of u's set) takes logarithmic time in total number of nodes



Implementation of Kruskal's Algorithm

Algorithm, rewritten with UNION-FIND:

- Create initial disjoint-set data structure, i.e. for each vertex v_i, store v_i as representative of its set
- Create empty forest F = {}
- Sort edges such that w.l.o.g. $w_1 < w_2 < \ldots < w_{|E|}$
- for each edge $e_i=\{u,v\}$ starting from i=1:
    - if FIND(u) ≠ FIND(v): # no cycle introduced?
        - $F = F \cup \{\{u,v\}\}$
        - UNION(u,v)
- return F

Back to Runtime Considerations

- Sorting of edges needs O(|E| log |E|)
- forest: **Disjoint-set data structure**
  - initialization: O(|V|)
  - log |V| to find out whether the minimum-cost edge {u,v} connects two sets (no cycle induced) or is within a set (cycle would be induced)
  - 2x FIND + potential UNION needs to be done O(|E|) times
  - total O(|E| log |V|)
- Overall: O(|E| log |E|)

Kruskal's Algorithm: Proof of Correctness

Two parts needed:

❶ Algo always produces a spanning tree

final F contains no cycle and is connected by definition ✓

❷ Algo always produces a *minimum* spanning tree

- argument by induction
- P: If *F* is forest at a given stage of the algorithm, then there is some minimum spanning tree that contains *F*.
- clearly true for F = (V, {})
- assume that P holds when new edge e is added to F and be T a MST that contains F
  - if e in T, fine
  - if e not in T: T + e has cycle C with edge f in C but not in F (otherwise e would have introduced a cycle in F)
    - now T – f + e is a tree with same weight as T (since T is a MST and f was not chosen to F)
    - hence T – f + e is MST including F + e (i.e. P holds) ✓

Conclusion Greedy Algorithms I

What we have seen so far:

- two problems where a greedy algorithm was optimal
  - money change
  - minimum spanning tree (Kruskal's algorithm)
- but also: greedy not always optimal
  - for some sets of coins for example

Obvious Question: when is greedy good?

Answer: if the problem is a matroid (no further details here)

From Wikipedia: [...] a matroid is a structure that captures and generalizes the notion of linear independence in vector spaces. There are many equivalent ways to define a matroid, the most significant being in terms of independent sets, bases, circuits, closed sets or flats, closure operators, and rank functions.

Conclusions Greedy Algorithms II

I hope it became clear...

...what a greedy algorithm is

...that it not always results in the optimal solution

...but that it does if and only if the problem is a matroid

2nd Intermediate Exam

Dynamic Programming

Dynamic Programming

Wikipedia:

“[...] **dynamic programming** is a method for solving a complex problem by breaking it down into a collection of simpler subproblems.”

But that’s not all:

- dynamic programming also makes sure that the subproblems are not solved too often but only once by keeping the solutions of simpler subproblems in memory (“trading space vs. time”)
- it is an exact method, i.e. in comparison to the greedy approach, it always solves a problem to optimality

Note:

the reason why the approach is called "dynamic programming" is historical: at the time of invention by Richard Bellman, no computer "program" existed

Two Properties Needed

Optimal Substructure

A solution can be constructed efficiently from optimal solutions of sub-problems

Overlapping Subproblems

Wikipedia: “[...] a problem is said to have **overlapping subproblems** if the problem can be broken down into subproblems which are reused several times or a recursive algorithm for the problem solves the same subproblem over and over rather than always generating new subproblems.”

Note: in case of optimal substructure but independent subproblems, often greedy algorithms are a good choice; in this case, dynamic programming is often called “divide and conquer” instead

Main Idea Behind Dynamic Programming

Main idea: solve larger subproblems by breaking them down to smaller, easier subproblems in a recursive manner

Typical Algorithm Design:

➊ decompose the problem into subproblems and think about how to solve a larger problem with the solutions of its subproblems

➋ specify how you compute the value of a larger problem recursively with the help of the optimal values of its subproblems ("Bellman equation")

➌ bottom-up solving of the subproblems (i.e. computing their optimal value), starting from the smallest by using the Bellman equality and a table structure to store the optimal values (top-down approach also possible, but less common)

➍ eventually construct the final solution (can be omitted if only the value of an optimal solution is sought)

Lecture Outline Dynamic Programming (DP)

What we will see:

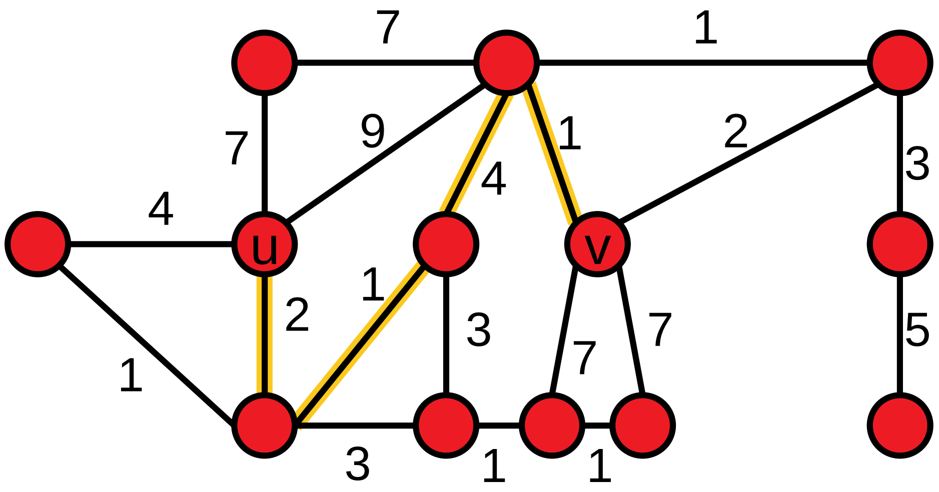
❶ Example 1: The All-Pairs Shortest Path Problem

❷ Example 2: The knapsack problem

Example 1: The Shortest Path Problem

Shortest Path problem:

Given a graph G=(V,E) with edge weights w_i for each edge e_i.
Find the shortest path from a vertex v to a vertex u, i.e., the path (v, $e_1=\{v, v_1\}$, v_1, ..., v_k, $e_k=\{v_k,u\}$, u) such that $w_1 + \ldots + w_k$ is minimized.



Obvious Applications

Google maps

Autonomous cars

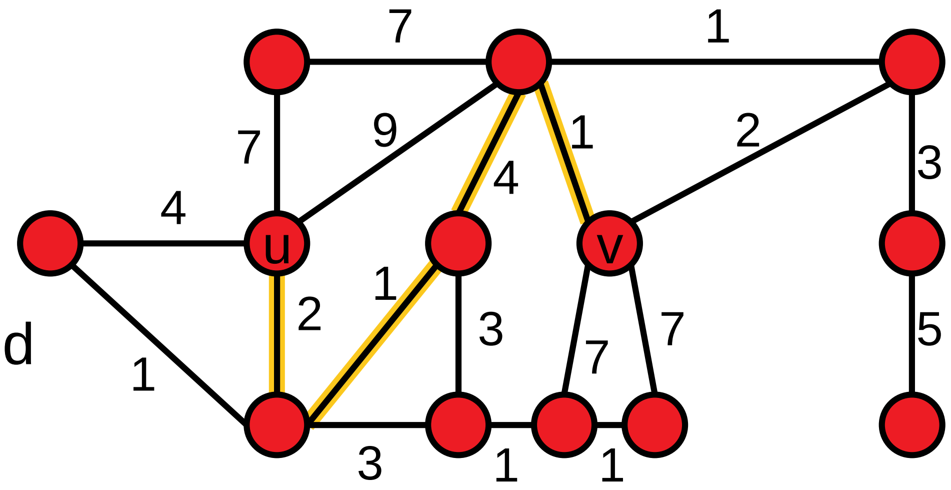
Finding routes for packages in a computer network

...

Example 1: The Shortest Path Problem

Shortest Path problem:

Given a graph G=(V,E) with edge weights w_i for each edge e_i. Find the shortest path from a vertex v to a vertex u, i.e., the path (v, e_1={v, v_1}, v_1, ..., v_k, e_k={v_k,u}, u) such that w_1 + ... + w_k is minimized.



Note:

We can often assume that the edge weights are stored in a distance matrix D of dimension |V|x|V| where an entry $D_{i,j}$ gives the weight between nodes i and j and “non-edges” are assigned a value of ∞

Why important? ⇨ determines input size

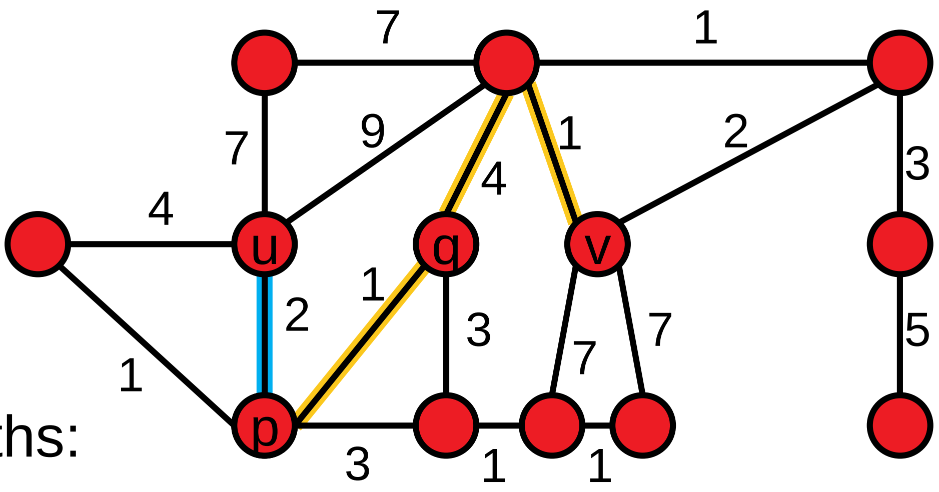
Opt. Substructure and Overlapping Subproblems

Optimal Substructure

The optimal path from u to v, if it contains another vertex p can be constructed by simply joining the optimal path from u to p with the optimal path from p to v.

Overlapping Subproblems

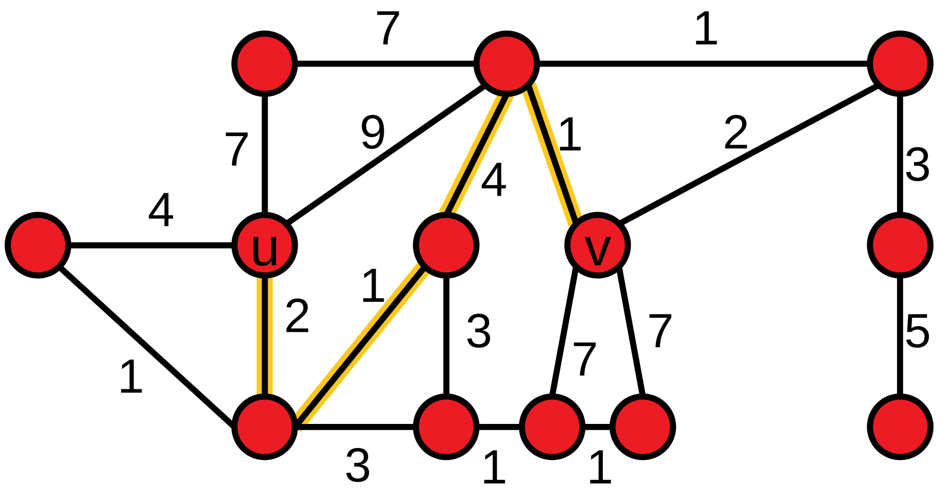
Optimal shortest sub-paths can be reused when computing longer paths: e.g. the optimal path from u to p is contained in the optimal path from u to q and in the optimal path from u to v.



The All Pairs Shortest Paths Problem

All Pairs Shortest Path problem:

Given a graph G=(V,E) with edge weights w_i for each edge e_i. Find the shortest path from each source vertex v to each other target vertex u, i.e., the paths (v, e_1={v, v_1}, v_1, ..., v_k, e_k={v_k,u}, u) such that $w_1 + \ldots + w_k$ is minimized for all pairs (u,v) in V^2.



The Algorithm of Robert Floyd (1962)

Idea:

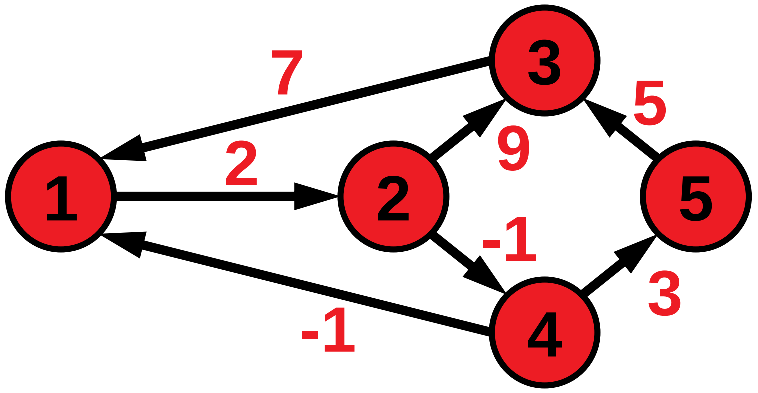
- if we knew that the shortest path between source and target goes through node v, we would be able to construct the optimal path from the shorter paths “source→v” and “v→target”
- subproblem P(k): compute all shortest paths where the intermediate nodes can be chosen from $v_1, ..., v_k$

AllPairsShortestPathFloyd(G, D)

```
▪ Init: for all $1 \leq i,j \leq |V|$: $dist(i,j) = D_{i,j}$
▪ For k = 1 to $|V|$        # solve subproblems P(k)
    ▪ for all pairs of nodes (i.e. $1 \leq i,j \leq |V|$):
        ▪ $dist(i,j) = \min \{ dist(i,j), dist(i,k) + dist(k,j) \}$
```

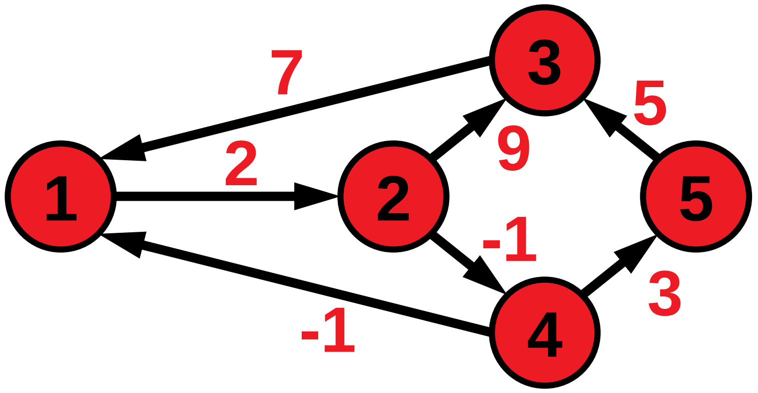
Note: Bernard Roy in 1959 and Stephen Warshall in 1962 essentially proposed the same algorithm independently.

Example



k=0	1	2	3	4	5
1					
2					
3					
4					
5					

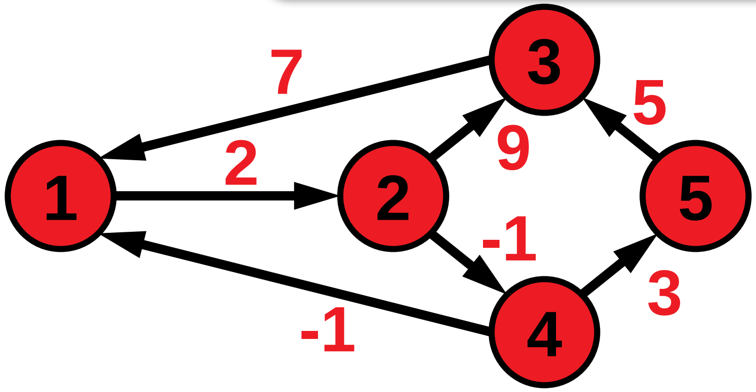
Example



k=0	1	2	3	4	5
1	∞	2	∞	∞	∞
2	∞	∞	9	-1	∞
3	7	∞	∞	∞	∞
4	-1	∞	∞	∞	3
5	∞	∞	5	∞	∞

Example

for all pairs of nodes (i.e. 1 ≤ i,j ≤ |V|):
dist(i,j) = min { dist(i,j), dist(i,k) + dist(k,j) }



allow 1 as intermediate node

k=0	1	2	3	4	5
1	∞	2	∞	∞	∞
2	∞	∞	9	-1	∞
3	7	∞	∞	∞	∞
4	-1	∞	∞	∞	3
5	∞	∞	5	∞	∞

k=1	1	2	3	4	5
1					
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Example

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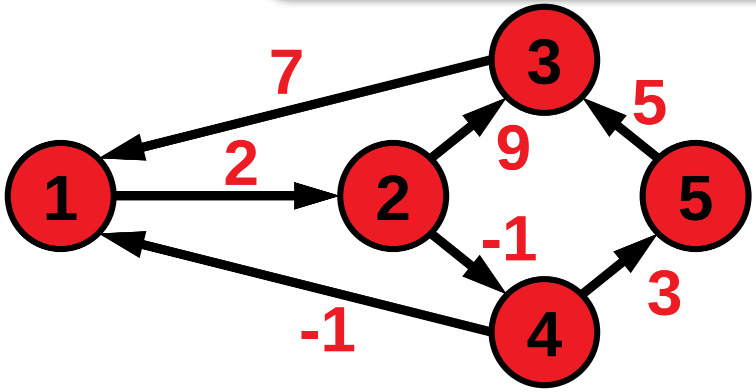

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4	-1	∞	∞	∞	3
5	∞	∞	5	∞	∞

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1					
2					
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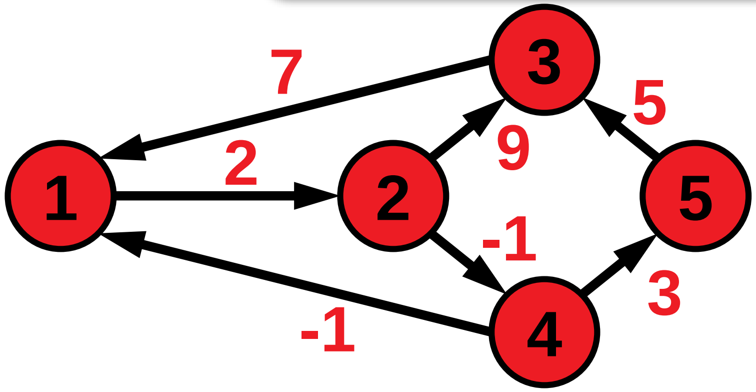

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4	-1	∞	∞	∞	3
5	∞	∞	5	∞	∞

k=1	1	2	3	4	5
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2					
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5					

Example

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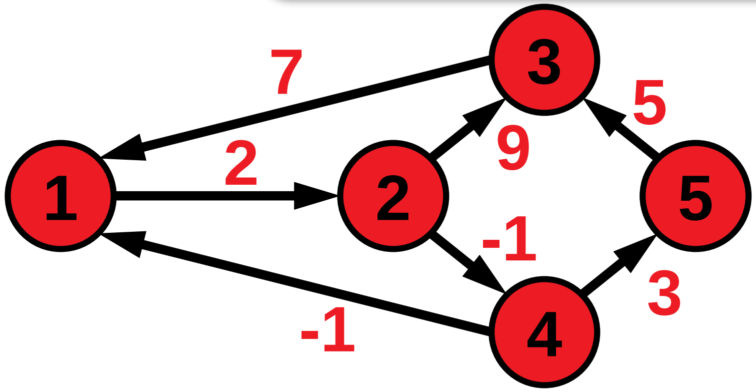

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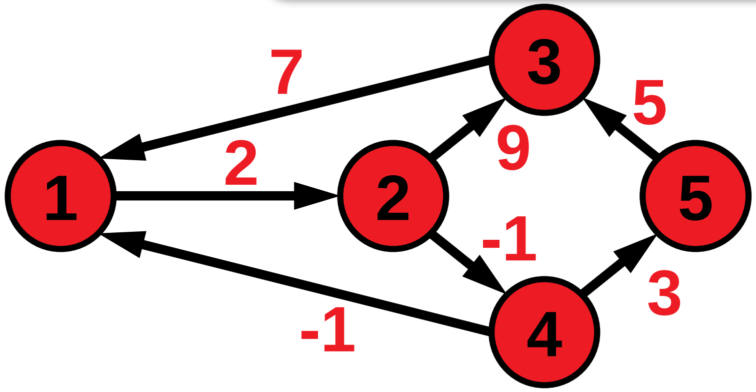
2	∞	∞	9	-1	∞
3	7	∞	∞	∞	∞
4	-1	∞	∞	∞	3
5	∞	∞	5	∞	∞

k=1	1	2	3	4	5
1					
2					
3		9			
4		1			
5					

Example

for all pairs of nodes (i.e. 1 ≤ i,j ≤ |V|):
dist(i,j) = min { dist(i,j), dist(i,k) + dist(k,j) }



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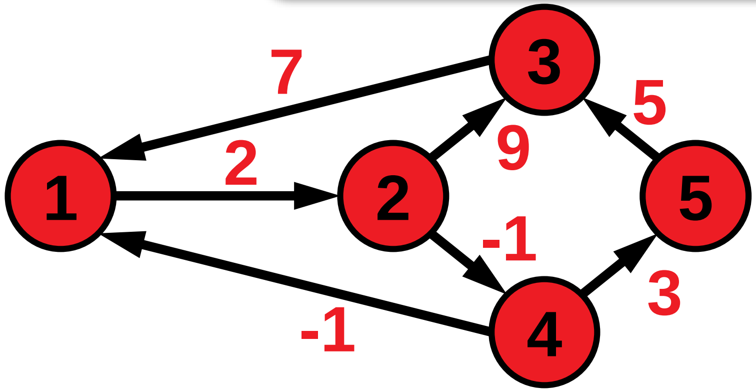
3	7	9	∞	∞	∞
4	-1	1	∞	∞	3
5	∞	∞	5	∞	∞

Example

for all pairs of nodes (i.e. 1 ≤ i,j ≤ |V|):
dist(i,j) = min { dist(i,j), dist(i,k) + dist(k,j) }



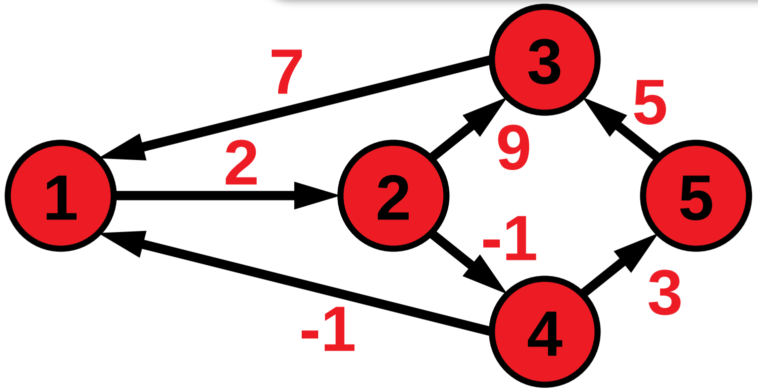
allow 1 & 2 as intermediate nodes

k=1	1	2	3	4	5
1	∞	2	∞	∞	∞
2	∞	∞	9	-1	∞
3	7	9	∞	∞	∞
4	-1	1	∞	∞	3
5	∞	∞	5	∞	∞

k=2	1	2	3	4	5
1	∞	2	∞	∞	∞
2	∞	∞	9	-1	∞
3	7	9	∞	∞	∞
4	-1	1	∞	∞	3
5	∞	∞	5	∞	∞

Example

for all pairs of nodes (i.e. 1 ≤ i,j ≤ |V|):
dist(i,j) = min { dist(i,j), dist(i,k) + dist(k,j) }



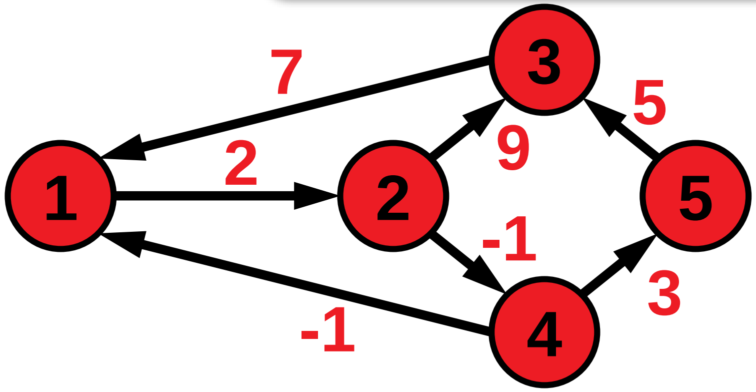
allow 1 & 2 as intermediate nodes

k=1	1	2	3	4	5
1	∞	2	∞	∞	∞
2	∞	∞	9	-1	∞
3	7	9	∞	∞	∞
4	-1	1	∞	∞	3
5	∞	∞	5	∞	∞

k=2	1	2	3	4	5
1	∞	2	∞	∞	∞
2	∞	∞	9	-1	∞
3	7	9	∞	∞	∞
4	-1	1	∞	∞	3
5	∞	∞	5	∞	∞

Example

for all pairs of nodes (i.e. 1 ≤ i,j ≤ |V|):
dist(i,j) = min { dist(i,j), dist(i,k) + dist(k,j) }



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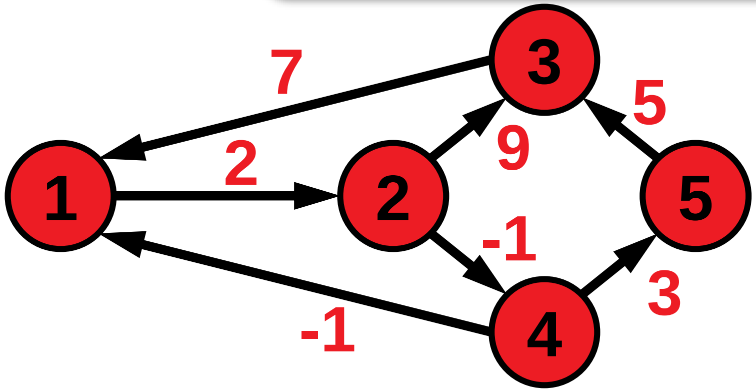
2	∞	∞	9	-1	∞
3	7	9	∞	∞	∞
4	-1	1	∞	∞	3
5	∞	∞	5	∞	∞

k=2	1	2	3	4	5
1	∞	2	11	1	∞
2	∞	∞	9	-1	∞
3	7	9	18	8	∞
4	-1	1	10	0	3
5	∞	∞	5	∞	∞

Example

for all pairs of nodes (i.e. 1 ≤ i,j ≤ |V|):
dist(i,j) = min { dist(i,j), dist(i,k) + dist(k,j) }



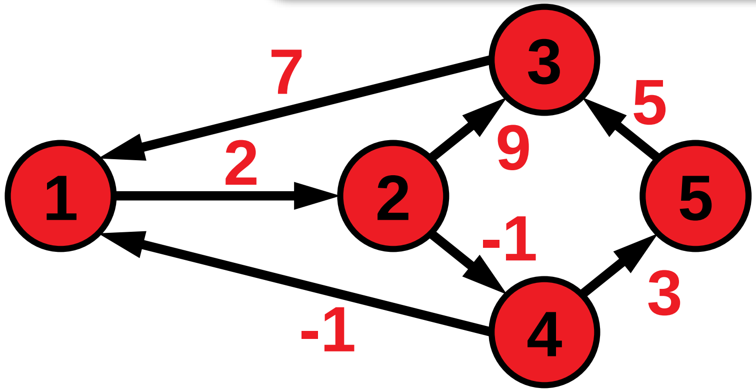
allow {1,2,3} as intermediate nodes

k=2	1	2	3	4	5
1	∞	2	11	1	∞
2	∞	∞	9	-1	∞
3	7	9	18	8	∞
4	-1	1	10	0	3
5	∞	∞	5	∞	∞

k=3	1	2	3	4	5
1	∞	2	11	1	∞
2	∞	∞	9	-1	∞
3	7	9	18	8	∞
4	-1	1	10	0	3
5	∞	∞	5	∞	∞

Example

for all pairs of nodes (i.e. 1 ≤ i,j ≤ |V|):
dist(i,j) = min { dist(i,j), dist(i,k) + dist(k,j) }



allow {1,2,3} as intermediate nodes

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4	-1	1	10	0	3
5	∞	∞	5	∞	∞

k=3	1	2	3	4	5
1			11		∞
2			9		∞
3	7	9	18	8	∞
4			10		3
5			5		∞

Example

for all pairs of nodes (i.e. 1 ≤ i,j ≤ |V|):
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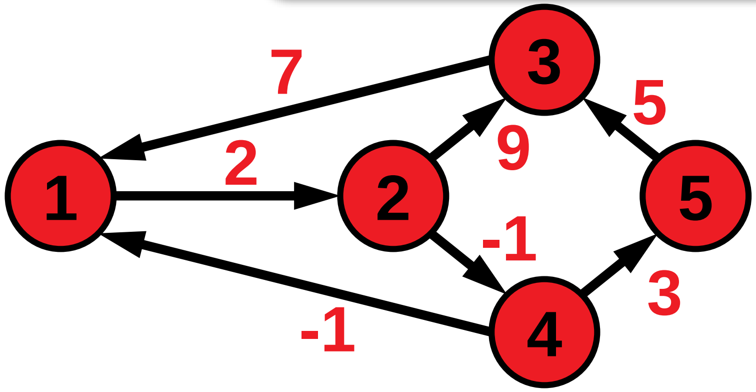

allow {1,2,3} as intermediate nodes

k=2	1	2	3	4	5
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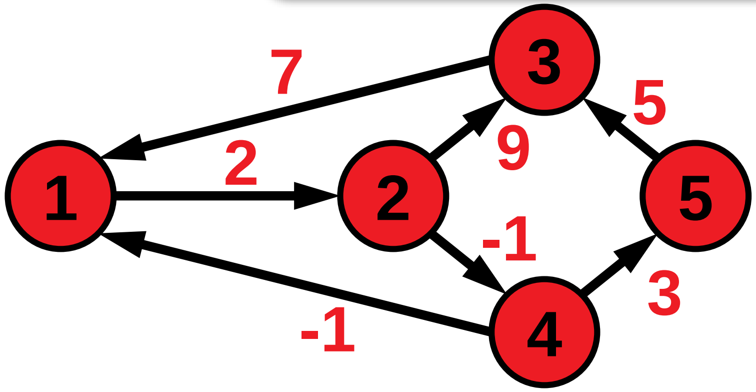
2	∞	∞	9	-1	∞
3	7	9	18	8	∞
4	-1	1	10	0	3
5	∞	∞	5	∞	∞

k=3	1	2	3	4	5
1	18	2	11	1	∞
2	16	18	9	-1	∞
3	7	9	18	8	∞
4	-1	1	10	0	3
5	12	14	5	13	∞

Example

for all pairs of nodes (i.e. $1 \le i,j \le |V|$):
dist(i,j) = min { dist(i,j), dist(i,k) + dist(k,j) }



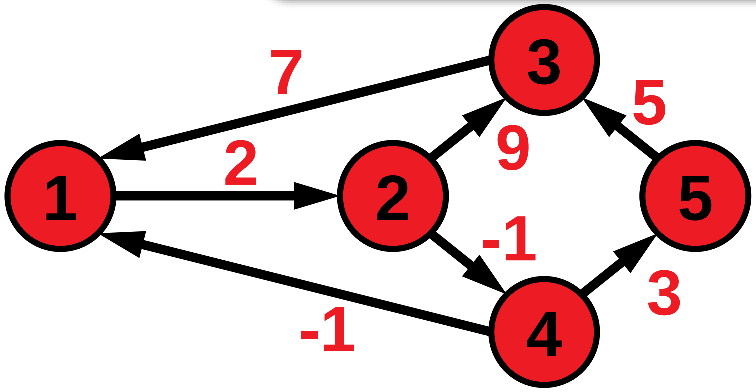
allow {1,2,3,4} as intermediate nodes

k=3	1	2	3	4	5
1	18	2	11	1	∞
2	16	18	9	-1	∞
3	7	9	18	8	∞
4	-1	1	10	0	3
5	12	14	5	13	∞

k=4	1	2	3	4	5
1	18	2	11	1	∞
2	16	18	9	-1	∞
3	7	9	18	8	∞
4	-1	1	10	0	3
5	12	14	5	13	∞

Example

for all pairs of nodes (i.e. 1 ≤ i,j ≤ |V|):
dist(i,j) = min { dist(i,j), dist(i,k) + dist(k,j) }



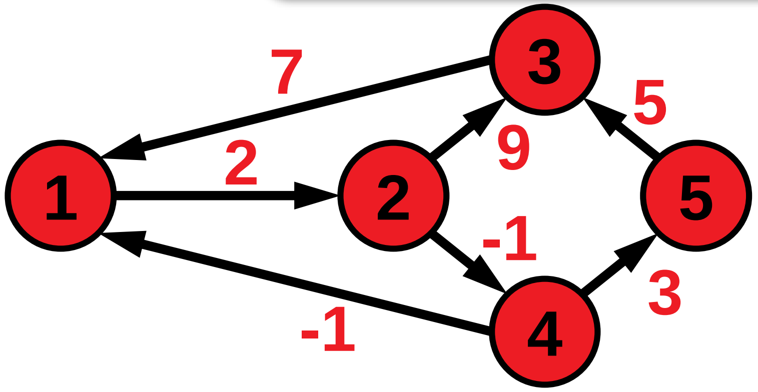
allow {1,2,3,4} as intermediate nodes

k=3	1	2	3	4	5
1	18	2	11	1	∞
2	16	18	9	-1	∞
3	7	9	18	8	∞
4	-1	1	10	0	3
5	12	14	5	13	∞

k=4	1	2	3	4	5
1				1	
2				-1	
3				8	
4	-1	1	10	0	3
5				13	

Example

for all pairs of nodes (i.e. 1 ≤ i,j ≤ |V|):
dist(i,j) = min { dist(i,j), dist(i,k) + dist(k,j) }



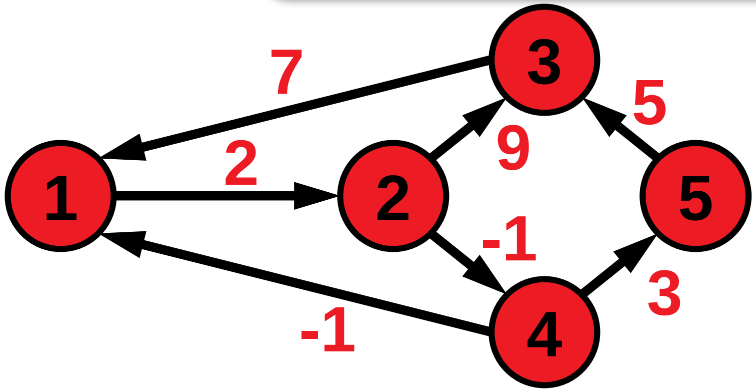
allow {1,2,3,4} as intermediate nodes

k=3	1	2	3	4	5
1	18	2	11	1	∞
2	16	18	9	-1	∞
3	7	9	18	8	∞
4	-1	1	10	0	3
5	12	14	5	13	∞

k=4	1	2	3	4	5
1	0	2	11	1	4
2	-2	0	9	-1	2
3	7	9	18	8	11
4	-1	1	10	0	3
5	12	14	5	13	16

Example

for all pairs of nodes (i.e. 1 ≤ i,j ≤ |V|):
dist(i,j) = min { dist(i,j), dist(i,k) + dist(k,j) }



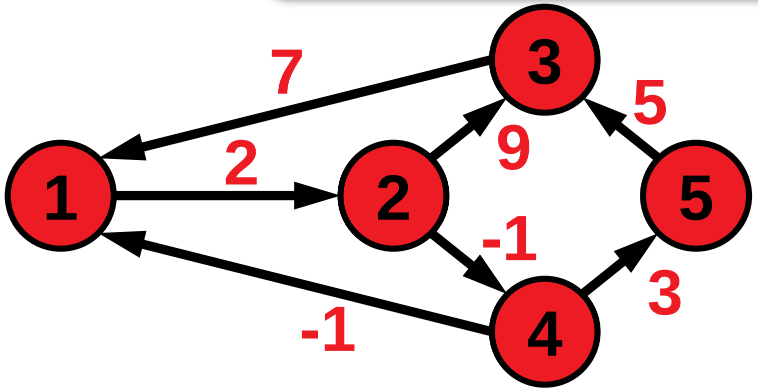
allow all nodes as intermediate nodes

k=4	1	2	3	4	5
1	0	2	11	1	4
2	-2	0	9	-1	2
3	7	9	18	8	11
4	-1	1	10	0	3
5	12	14	5	13	16

k=5	1	2	3	4	5
1	0	2	11	1	4
2	-2	0	9	-1	2
3	7	9	18	8	11
4	-1	1	10	0	3
5	12	14	5	13	16

Example

for all pairs of nodes (i.e. 1 ≤ i,j ≤ |V|):
dist(i,j) = min { dist(i,j), dist(i,k) + dist(k,j) }



allow all nodes as intermediate nodes

k=4	1	2	3	4	5
1	0	2	11	1	4
2	-2	0	9	-1	2
3	7	9	18	8	11
4	-1	1	10	0	3
5	12	14	5	13	16

k=5	1	2	3	4	5
1	0	2	9	1	4
2	-2	0	7	-1	2
3	7	9	16	8	11
4	-1	1	8	0	3
5	12	14	5	13	16

Runtime Considerations and Correctness

$O(|V|^3)$ easy to show

- $O(|V|^2)$ many distances need to be updated $O(|V|)$ times

Correctness

- given by the Bellman equation

  dist(i,j) = min { dist(i,j), dist(i,k) + dist(k,j) }

- only correct if cycles do not have negative total weight (can be checked in final distance matrix if diagonal elements are negative)

But How Can We Actually Construct the Paths?

- Construct matrix of predecessors P alongside distance matrix
- $P_{i,j}(k)$ = predecessor of node j on path from i to j (at algo. step k)
- no extra costs (asymptotically)

$$P_{i,j}(0) = \begin{cases} 0 & \text{if } i = j \text{ or } d_{i,j} = \infty \\ i & \text{in all other cases} \end{cases}$$

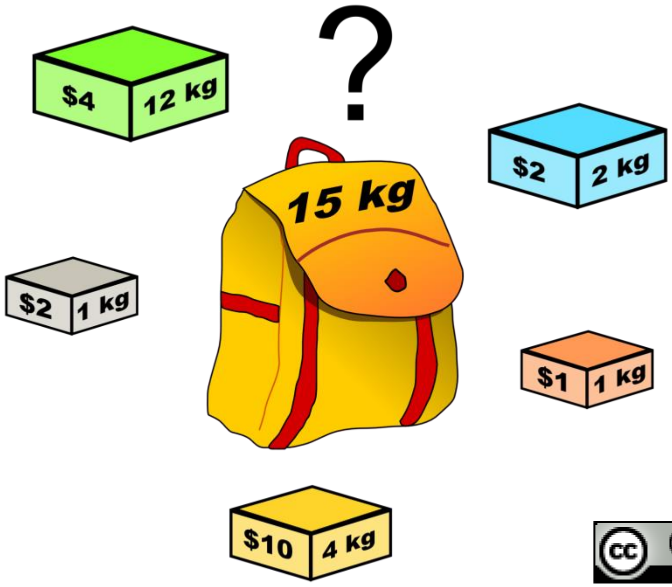
$$P_{i,j}(k) = \begin{cases} P_{i,j}(k-1) & \text{if } \mathrm{dist}(i,j) \leq \mathrm{dist}(i,k) + \mathrm{dist}(k,j) \\ P_{k,j}(k-1) & \text{if } \mathrm{dist}(i,j) > \mathrm{dist}(i,k) + \mathrm{dist}(k,j) \end{cases}$$

Example 2: The Knapsack Problem (KP)

Knapsack Problem

$$\max. \sum_{j=1}^{n} p_j x_j \text{ with } x_j \in \{0,1\}$$

$$\text{s.t.} \sum_{j=1}^{n} w_j x_j \leq W$$



Opt. Substructure and Overlapping Subproblems

Consider the following subproblem:

$P(i,j)$: optimal profit when packing the first i items into a knapsack of size j

Optimal Substructure

The optimal choice of whether taking item i or not can be made easily for a knapsack of weight j if we know the optimal choice for items $1 \ldots i-1$:

$$P(i,j) = \begin{cases} 0 & \text{if } i = 0 \text{ or } j = 0 \\ P(i-1,j) & \text{if } w_i > j \\ \max\{P(i-1,j), p_i + P(i-1, j-w_i)\} & \text{if } w_i \leq j \end{cases}$$

Overlapping Subproblems

a recursive implementation of the Bellman equation is simple, but the $P(i,j)$ might need to be computed more than once!

Dynamic Programming Approach to the KP

To circumvent computing the subproblems more than once, we can store their results (in a matrix for example)...

knapsack weight $\longrightarrow$

items $\downarrow$

P(i,j)	0	1	2	3	...			W-1	W
0									
1					P(i,j)				
2									
...									
n-1									
n									

best achievable profit with items 1...i and a knapsack of size j

Dynamic Programming Approach to the KP

Example instance with 5 items with weights and profits (5,4), (7,10), (2,3), (4,5), and (3,3). Weight restriction is W=11.

knapsack weight $\longrightarrow$

items $\downarrow$

P(i,j)	0	1	2	3	4	5	6	7	8	9	10	11
0												
1												
2												
3												
4												
5												

initialization:
$P(i,j) = 0$ if $i = 0$ or $j = 0$

Dynamic Programming Approach to the KP

Example instance with 5 items with weights and profits (5,4), (7,10), (2,3), (4,5), and (3,3). Weight restriction is W=11.

knapsack weight $\longrightarrow$

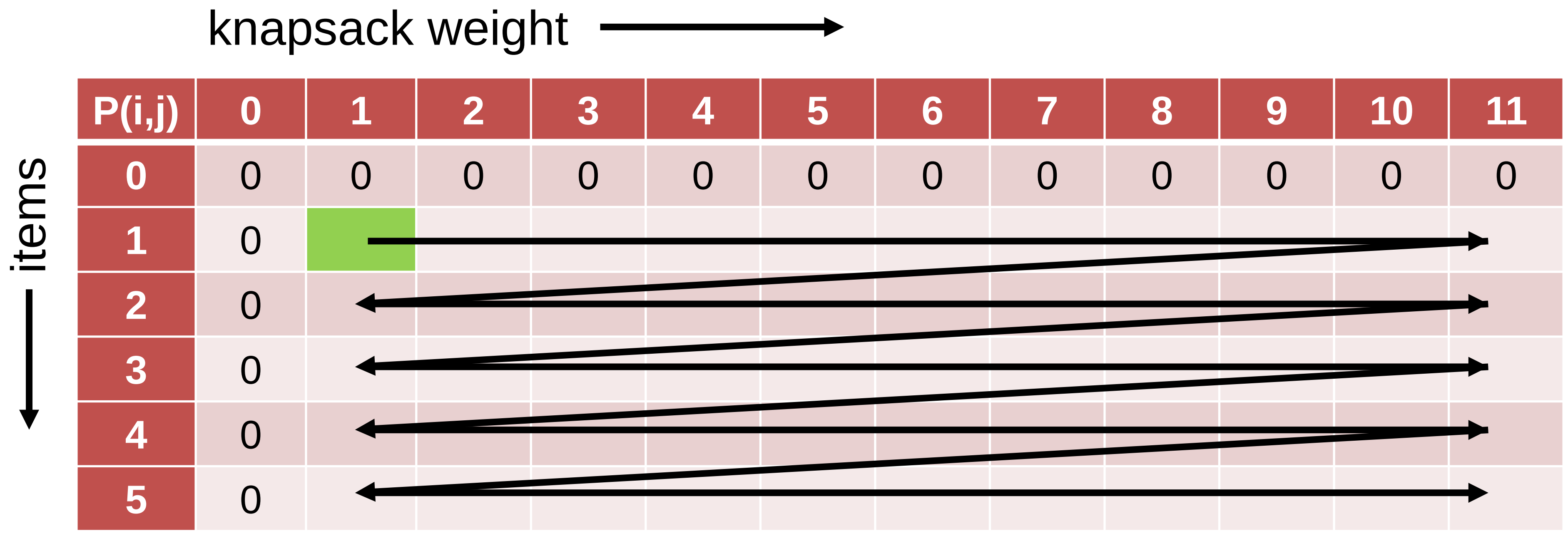
items $\downarrow$

P(i,j)	0	1	2	3	4	5	6	7	8	9	10	11
0	0	0	0	0	0	0	0	0	0	0	0	0
1	0											
2	0											
3	0											
4	0											
5	0											

initialization:
$P(i,j) = 0$ if $i = 0$ or $j = 0$

Dynamic Programming Approach to the KP

Example instance with 5 items with weights and profits $(5,4)$, $(7,10)$, $(2,3)$, $(4,5)$, and $(3,3)$. Weight restriction is $W = 11$.



P(i,j)	0	1	2	3	4	5	6	7	8	9	10	11
0	0	0	0	0	0	0	0	0	0	0	0	0
1	0	🟩										
2	0											
3	0											
4	0											
5	0											

```
for $i = 1$ to $n$:
        for $j = 1$ to $W$:
```

$$P(i,j) = \begin{cases} P(i-1,j) & \text{if } w_i > j \\ \max\{P(i-1,j), p_i + P(i-1,j-w_i)\} & \text{if } w_i \le j \end{cases}$$

Dynamic Programming Approach to the KP

Example instance with 5 items with weights and profits $(5,4)$, $(7,10)$, $(2,3)$, $(4,5)$, and $(3,3)$. Weight restriction is $W = 11$.

knapsack weight $\longrightarrow$

items $\downarrow$

P(i,j)	0	1	2	3	4	5	6	7	8	9	10	11
0	0	0	0	0	0	0	0	0	0	0	0	0
1	0	0										
2	0											
3	0											
4	0											
5	0											

```
for $i = 1$ to $n$:
        for $j = 1$ to $W$:
                $P(i,j) = \begin{cases} P(i-1,j) & \text{if } w_i > j \\ \max\{P(i-1,j), p_i + P(i-1,j-w_i)\} & \text{if } w_i \leq j \end{cases}$
```

Dynamic Programming Approach to the KP

Example instance with 5 items with weights and profits $(5,4)$, $(7,10)$, $(2,3)$, $(4,5)$, and $(3,3)$. Weight restriction is $W = 11$.

knapsack weight $\longrightarrow$

items $\downarrow$

P(i,j)	0	1	2	3	4	5	6	7	8	9	10	11
0	0	0	0	0	0	0	0	0	0	0	0	0
1	0	0	0									
2	0											
3	0											
4	0											
5	0											

```
for $i = 1$ to $n$:
    for $j = 1$ to $W$:
```

$$P(i,j) = \begin{cases} P(i-1,j) & \text{if } w_i > j \\ \max\{P(i-1,j), p_i + P(i-1,j-w_i)\} & \text{if } w_i \leq j \end{cases}$$

Dynamic Programming Approach to the KP

Example instance with 5 items with weights and profits $(5,4)$, $(7,10)$, $(2,3)$, $(4,5)$, and $(3,3)$. Weight restriction is $W = 11$.

knapsack weight $\longrightarrow$

items $\downarrow$

P(i,j)	0	1	2	3	4	5	6	7	8	9	10	11
0	0	0	0	0	0	0	0	0	0	0	0	0
1	0	0	0	0	0							
2	0											
3	0											
4	0											
5	0											

```
for $i = 1$ to $n$:
        for $j = 1$ to $W$:
```

$$P(i,j) = \begin{cases} P(i-1,j) & \text{if } w_i > j \\ \max\{P(i-1,j), p_i + P(i-1,j-w_i)\} & \text{if } w_i \le j \end{cases}$$

Dynamic Programming Approach to the KP

Example instance with 5 items with weights and profits $(5,4)$, $(7,10)$, $(2,3)$, $(4,5)$, and $(3,3)$. Weight restriction is $W = 11$.

knapsack weight $\longrightarrow$

items $\downarrow$

P(i,j)	0	1	2	3	4	5	6	7	8	9	10	11
0	0	0	0	0	0	0	0	0	0	0	0	0
1	0	0	0	0	0	4						
2	0											
3	0											
4	0											
5	0											

$+p_1(= 4)$

```
for $i = 1$ to $n$:
    for $j = 1$ to $W$:
        $P(i,j) = \begin{cases} P(i-1,j) & \text{if } w_i > j \\ \max\{P(i-1,j), p_i + P(i-1,j-w_i)\} & \text{if } w_i \le j \end{cases}$
```

Dynamic Programming Approach to the KP

Example instance with 5 items with weights and profits $(5,4)$, $(7,10)$, $(2,3)$, $(4,5)$, and $(3,3)$. Weight restriction is $W = 11$.

knapsack weight $\longrightarrow$

items $\downarrow$

P(i,j)	0	1	2	3	4	5	6	7	8	9	10	11
0	0	0	0	0	0	0	0	0	0	0	0	0
1	0	0	0	0	0	4	🟩 4					
2	0											
3	0											
4	0											
5	0											

$+p_1(= 4)$

```
for $i = 1$ to $n$:
        for $j = 1$ to $W$:
```

$$P(i,j) = \begin{cases} P(i-1,j) & \text{if } w_i > j \\ \max\{P(i-1,j), p_i + P(i-1, j-w_i)\} & \text{if } w_i \leq j \end{cases}$$

Dynamic Programming Approach to the KP

Example instance with 5 items with weights and profits $(5,4)$, $(7,10)$, $(2,3)$, $(4,5)$, and $(3,3)$. Weight restriction is $W = 11$.

knapsack weight $\longrightarrow$

items $\downarrow$

P(i,j)	0	1	2	3	4	5	6	7	8	9	10	11
0	0	0	0	0	0	0	0	0	0	0	0	0
1	0	0	0	0	0	4	4	4	4	4	4	4
2	0											
3	0											
4	0											
5	0											

```
for $i = 1$ to $n$:
    for $j = 1$ to $W$:
        $P(i,j) = \begin{cases} P(i-1,j) & \text{if } w_i > j \\ \max\{P(i-1,j), p_i + P(i-1,j-w_i)\} & \text{if } w_i \leq j \end{cases}$
```

Dynamic Programming Approach to the KP

Example instance with 5 items with weights and profits $(5,4)$, $(7,10)$, $(2,3)$, $(4,5)$, and $(3,3)$. Weight restriction is $W = 11$.

knapsack weight $\longrightarrow$

items $\downarrow$

P(i,j)	0	1	2	3	4	5	6	7	8	9	10	11
0	0	0	0	0	0	0	0	0	0	0	0	0
1	0	0	0	0	0	4	4	4	4	4	4	4
2	0	0	0	0	0	4	4					
3	0											
4	0											
5	0											

```
for $i = 1$ to $n$:
        for $j = 1$ to $W$:
$$P(i,j) = \begin{cases} P(i-1,j) & \text{if } w_i > j \\ \max\{P(i-1,j), p_i + P(i-1,j-w_i)\} & \text{if } w_i \leq j \end{cases}$$
```

Dynamic Programming Approach to the KP

Example instance with 5 items with weights and profits $(5,4)$, $(7,10)$, $(2,3)$, $(4,5)$, and $(3,3)$. Weight restriction is $W = 11$.

knapsack weight $\longrightarrow$

items $\downarrow$

P(i,j)	0	1	2	3	4	5	6	7	8	9	10	11
0	0	0	0	0	0	0	0	0	0	0	0	0
1	0	0	0	0	0	4	4	4	4	4	4	4
2	0	0	0	0	0	4	4	10				
3	0											
4	0											
5	0											

$+p_2(= 10)$

```
for $i = 1$ to $n$:
    for $j = 1$ to $W$:
```

$$P(i,j) = \begin{cases} P(i-1,j) & \text{if } w_i > j \\ \max\{P(i-1,j), p_i + P(i-1, j-w_i)\} & \text{if } w_i \leq j \end{cases}$$

Dynamic Programming Approach to the KP

Example instance with 5 items with weights and profits $(5,4)$, $(7,10)$, $(2,3)$, $(4,5)$, and $(3,3)$. Weight restriction is $W = 11$.

knapsack weight $\longrightarrow$

items $\downarrow$

P(i,j)	0	1	2	3	4	5	6	7	8	9	10	11
0	0	0	0	0	0	0	0	0	0	0	0	0
1	0	0	0	0	0	4	4	4	4	4	4	4
2	0	0	0	0	0	4	4	10	10	10	10	10
3	0											
4	0											
5	0											

```
for $i = 1$ to $n$:
        for $j = 1$ to $W$:
```

$$P(i,j) = \begin{cases} P(i-1,j) & \text{if } w_i > j \\ \max\{P(i-1,j), p_i + P(i-1,j-w_i)\} & \text{if } w_i \leq j \end{cases}$$

Dynamic Programming Approach to the KP

Example instance with 5 items with weights and profits $(5,4)$, $(7,10)$, $(2,3)$, $(4,5)$, and $(3,3)$. Weight restriction is $W = 11$.

knapsack weight $\longrightarrow$

items $\downarrow$

P(i,j)	0	1	2	3	4	5	6	7	8	9	10	11
0	0	0	0	0	0	0	0	0	0	0	0	0
1	0	0	0	0	0	4	4	4	4	4	4	4
2	0	0	0	0	0	4	4	10	10	10	10	10
3	0	0	3	3	3							
4	0											
5	0											

```
for $i = 1$ to $n$:
        for $j = 1$ to $W$:
                $P(i,j) = \begin{cases} P(i-1,j) & \text{if } w_i > j \\ \max\{P(i-1,j), p_i + P(i-1,j-w_i)\} & \text{if } w_i \leq j \end{cases}$
```

Dynamic Programming Approach to the KP

Example instance with 5 items with weights and profits $(5,4)$, $(7,10)$, $(2,3)$, $(4,5)$, and $(3,3)$. Weight restriction is $W = 11$.

knapsack weight $\longrightarrow$

items $\downarrow$

P(i,j)	0	1	2	3	4	5	6	7	8	9	10	11
0	0	0	0	0	0	0	0	0	0	0	0	0
1	0	0	0	0	0	4	4	4	4	4	4	4
2	0	0	0	0	0	4	4	10	10	10	10	10
3	0	0	3	3	3	4						
4	0											
5	0											

$+p_3(=3)$

```
for $i = 1$ to $n$:
        for $j = 1$ to $W$:
                $P(i,j) = \begin{cases} P(i-1,j) & \text{if } w_i > j \\ \max\{P(i-1,j), p_i + P(i-1,j-w_i)\} & \text{if } w_i \le j \end{cases}$
```

Dynamic Programming Approach to the KP

Example instance with 5 items with weights and profits $(5,4)$, $(7,10)$, $(2,3)$, $(4,5)$, and $(3,3)$. Weight restriction is $W = 11$.

knapsack weight $\longrightarrow$

items $\downarrow$

P(i,j)	0	1	2	3	4	5	6	7	8	9	10	11
0	0	0	0	0	0	0	0	0	0	0	0	0
1	0	0	0	0	0	4	4	4	4	4	4	4
2	0	0	0	0	0	4	4	10	10	10	10	10
3	0	0	3	3	3 $+p_3(= 3)$	4	🟩 4					
4	0											
5	0											

```
for $i = 1$ to $n$:
        for $j = 1$ to $W$:
```

$$P(i,j) = \begin{cases} P(i-1,j) & \text{if } w_i > j \\ \max\{P(i-1,j), p_i + P(i-1, j-w_i)\} & \text{if } w_i \leq j \end{cases}$$

Dynamic Programming Approach to the KP

Example instance with 5 items with weights and profits $(5{,}4)$, $(7{,}10)$, $(2{,}3)$, $(4{,}5)$, and $(3{,}3)$. Weight restriction is $W = 11$.

knapsack weight $\longrightarrow$

items $\downarrow$

P(i,j)	0	1	2	3	4	5	6	7	8	9	10	11
0	0	0	0	0	0	0	0	0	0	0	0	0
1	0	0	0	0	0	4	4	4	4	4	4	4
2	0	0	0	0	0	4	4	10	10	10	10	10
3	0	0	3	3	3	4	4	🟩 10	etc.			
4	0											
5	0											

$+p_3(=3)$

```
for $i = 1$ to $n$:
    for $j = 1$ to $W$:
        $P(i,j) = \begin{cases} P(i-1,j) & \text{if } w_i > j \\ \max\{P(i-1,j),\, p_i + P(i-1,j-w_i)\} & \text{if } w_i \leq j \end{cases}$
```

Dynamic Programming Approach to the KP

Example instance with 5 items with weights and profits $(5,4)$, $(7,10)$, $(2,3)$, $(4,5)$, and $(3,3)$. Weight restriction is $W = 11$.

knapsack weight $\longrightarrow$

items $\downarrow$

P(i,j)	0	1	2	3	4	5	6	7	8	9	10	11
0	0	0	0	0	0	0	0	0	0	0	0	0
1	0	0	0	0	0	4	4	4	4	4	4	4
2	0	0	0	0	0	4	4	10	10	10	10	10
3	0	0	3	3	3	4	4	10	10	13	13	13
4	0	0	3	3	5	5	8	10	10	13	13	15
5	0	0	3	3	5	6	8	10	10	13	13	15

```
for $i = 1$ to $n$:
    for $j = 1$ to $W$:
```

$$P(i,j) = \begin{cases} P(i-1,j) & \text{if } w_i > j \\ \max\{P(i-1,j), p_i + P(i-1, j-w_i)\} & \text{if } w_i \leq j \end{cases}$$

Dynamic Programming Approach to the KP

Example instance with 5 items with weights and profits $(5,4)$, $(7,10)$, $(2,3)$, $(4,5)$, and $(3,3)$. Weight restriction is $W = 11$.

knapsack weight $\longrightarrow$

items $\downarrow$

P(i,j)	0	1	2	3	4	5	6	7	8	9	10	11
0	0	0	0	0	0	0	0	0	0	0	0	0
1	0	0	0	0	0	4	4	4	4	4	4	4
2	0	0	0	0	0	4	4	10	10	10	10	10
3	0	0	3	3	3	4	4	10	10	13	13	13
4	0	0	3	3	5	5	8	10	10	13	13	15
5	0	0	3	3	5	6	8	10	10	13	13	**15**

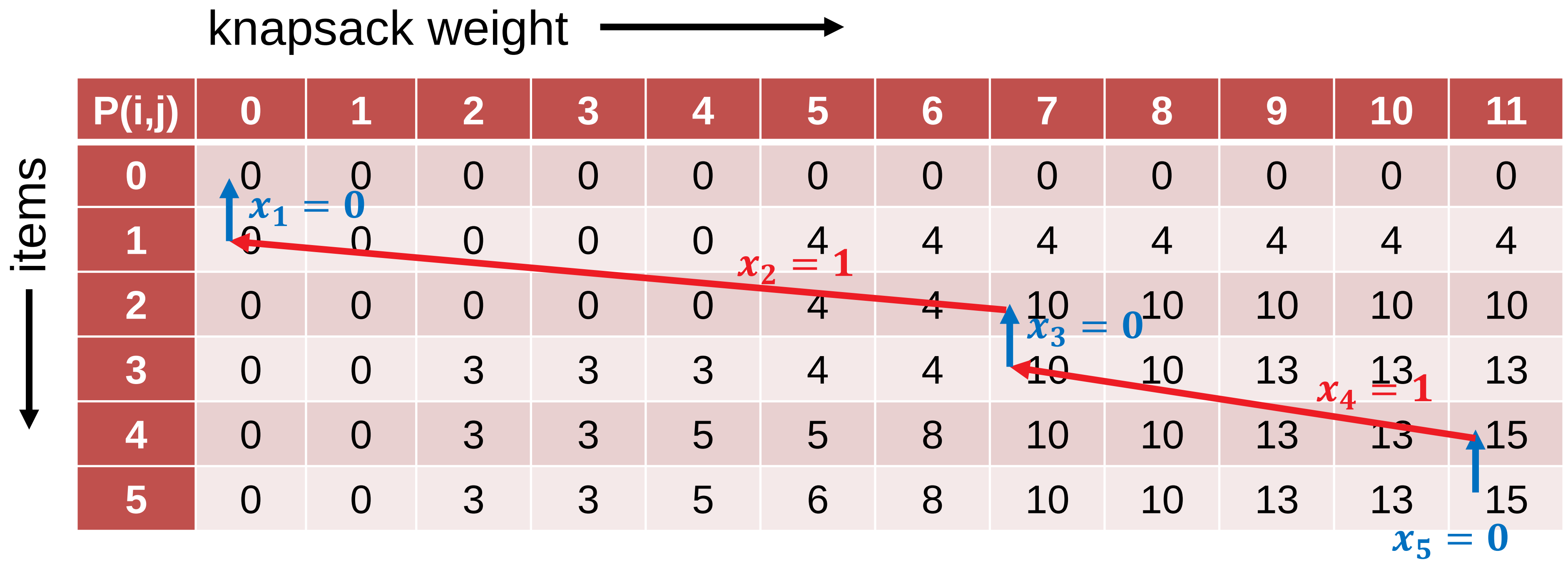
```
for $i = 1$ to $n$:
        for $j = 1$ to $W$:
```

$$P(i,j) = \begin{cases} P(i-1,j) & \text{if } w_i > j \\ \max\{P(i-1,j), p_i + P(i-1,j-w_i)\} & \text{if } w_i \leq j \end{cases}$$

Dynamic Programming Approach to the KP

Question: How to obtain the actual packing?

Answer: we just need to remember where the $\max$ came from!



P(i,j)	0	1	2	3	4	5	6	7	8	9	10	11
0	0	0	0	0	0	0	0	0	0	0	0	0
1	0	0	0	0	0	4	4	4	4	4	4	4
2	0	0	0	0	0	4	4	10	10	10	10	10
3	0	0	3	3	3	4	4	10	10	13	13	13
4	0	0	3	3	5	5	8	10	10	13	13	15
5	0	0	3	3	5	6	8	10	10	13	13	15

```
for $i = 1$ to $n$:
        for $j = 1$ to $W$:
```

$$P(i,j) = \begin{cases} P(i-1,j) & \text{if } w_i > j \\ \max\{P(i-1,j), p_i + P(i-1,j-w_i)\} & \text{if } w_i \leq j \end{cases}$$

Conclusions

I hope it became clear...

...what the algorithm design ideas of dynamic programming are

...and for which problem types it is supposed to be suitable

The following slides have not been discussed during the lecture and, thus, will not be part of the final exam.

(Randomized) Search Heuristics

Motivation General Search Heuristics

- often, problem complicated and not much time available to develop a problem-specific algorithm
- search heuristics are a good choice:
  - relatively easy to implement
  - easy to adapt/change/improve
    - e.g. when the problem formulation changes in an early product design phase
    - or when slightly different problems need to be solved over time
- randomized/stochastic algorithms are a good choice because they are robust to noise

Lecture Outline Randomized Search Heuristics

Which algorithms will we touch?

❶ Randomized Local Search (RLS)

❷ Variable Neighborhood Search (VNS)

❸ Tabu Search (TS)

❹ Evolutionary Algorithms (EAs)

Neighborhoods

For most (stochastic) search heuristics, we need to define a *neighborhood structure*

- which search points are close to each other?

Example: k-bit flip / Hamming distance k neighborhood

- search space: bitstrings of length n ($\Omega=\{0,1\}^n$)
- two search points are neighbors if their Hamming distance is k
- in other words: x and y are neighbors if we can flip exactly k bits in x to obtain y
- 0001001101 is neighbor of
  0001000101 for k=1
  0101000101 for k=2
  1101000101 for k=3

Neighborhoods II

Example: possible neighborhoods for the knapsack problem

- search space again bitstrings of length n ($\Omega=\{0,1\}^n$)
- Hamming distance 1 neighborhood:
  - add an item or remove it from the packing
- replacing 2 items neighborhood:
  - replace one chosen item with an unchosen one
  - makes only sense in combination with other neighborhoods because the number of items stays constant
- Hamming distance 2 neighborhood on the contrary:
  - allows to change 2 arbitrary items, e.g.
    - add 2 new items
    - remove 2 chosen items
    - or replace one chosen item with an unchosen one

Randomized Local Search (RLS)

Idea behind (Randomized) Local Search:

- explore the local neighborhood of the current solution (randomly)

Pure Random Search:

- go to randomly chosen neighbor

First Improvement Local Search:

- go to first (randomly) chosen neighbor which is better

Best Improvement strategy:

- always go to the best neighbor
- not random anymore
- computationally expensive if neighborhood large

Variable Neighborhood Search

Main Idea: [Mladenovic and P. Hansen, 1997]

- change the neighborhood from time to time
  - local optima are not the same for different neighborhood operators
  - but often close to each other
  - global optimum is local optimum for all neighborhoods
- rather a framework than a concrete algorithm
  - e.g. deterministic and stochastic neighborhood changes
- typically combined with (i) first improvement, (ii) a random order in which the neighbors are visited and (iii) restarts

N. Mladenovic and P. Hansen (1997). "Variable neighborhood search". Computers and Operations Research 24 (11): 1097–1100.

Tabu Search

Disadvantages of local searches (with or without varying neighborhoods)

- they get stuck in local optima
- have problems to traverse large plateaus of equal objective function value ("random walk")

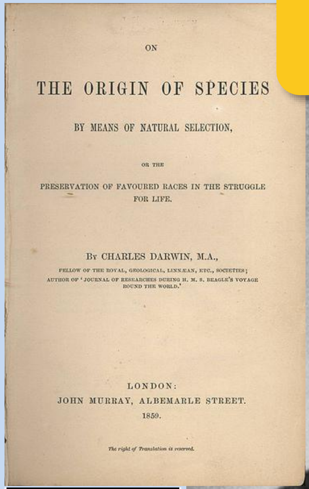
Tabu search addresses these by

- allowing worsening moves if all neighbors are explored
- introducing a tabu list of temporarily not allowed moves
- those restricted moves are
  - problem-specific and
  - can be specific solutions or not permitted "search directions" such as "don't include this edge anymore" or "do not flip this specific bit"
- the tabu list is typically restricted in size and after a while, restricted moves are permitted again

Stochastic Optimization Algorithms

One class of (bio-inspired) stochastic optimization algorithms: Evolutionary Algorithms (EAs)

1859



ON

THE ORIGIN OF SPECIES

BY MEANS OF NATURAL SELECTION,

OR THE

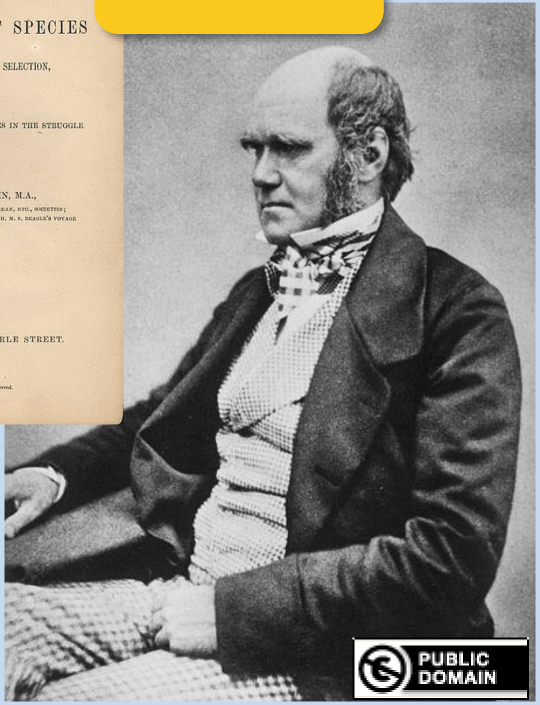
PRESERVATION OF FAVOURED RACES IN THE STRUGGLE FOR LIFE.

BY CHARLES DARWIN, M.A.,

FELLOW OF THE ROYAL, GEOLOGICAL, LINNÆAN, ETC., SOCIETIES;
AUTHOR OF 'JOURNAL OF RESEARCHES DURING H. M. S. BEAGLE'S VOYAGE ROUND THE WORLD.'

LONDON:
JOHN MURRAY, ALBEMARLE STREET.
1859.

The right of Translation is reserved.

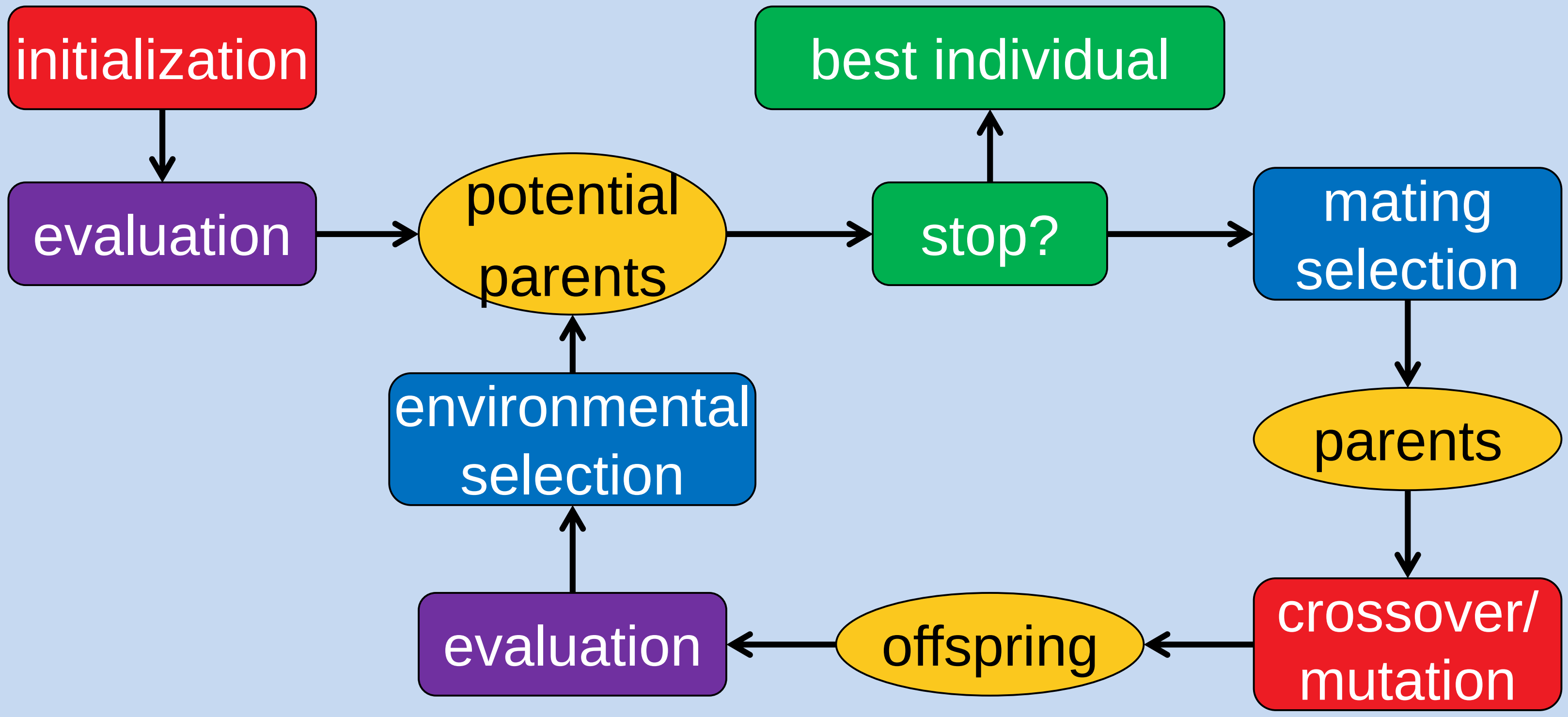


- Class of optimization algorithms originally inspired by the idea of biological evolution
- selection, mutation, recombination

Metaphors

Classical Optimization	Evolutionary Computation
variables or parameters	variables or chromosomes
candidate solution vector of decision variables / design variables / object variables	individual, offspring, parent
set of candidate solutions	population
objective function loss function cost function error function	fitness function
iteration	generation

Generic Framework of an EA



stochastic operators

“Darwinism”

stopping criteria

Important:
representation (search space)

The Historic Roots of EAs

Genetic Algorithms (GA)

J. Holland 1975 and D. Goldberg (USA)

$$\Omega = \{0,1\}^n$$

Evolution Strategies (ES)

I. Rechenberg and H.P. Schwefel, 1965 (Berlin)

$$\Omega = \mathbb{R}^n$$

Evolutionary Programming (EP)

L.J. Fogel 1966 (USA)

Genetic Programming (GP)

J. Koza 1990 (USA)

$$\Omega = \text{space of all programs}$$

nowadays one umbrella term: evolutionary algorithms

Genotype – Phenotype mapping

The genotype – phenotype mapping

- related to the question: how to come up with a fitness ("quality") of each individual from the representation?
- related to DNA vs. actual animal (which then has a fitness)

fitness of an individual not always = f(x)

- include constraints
- include diversity
- others
- but needed: always a total order on the solutions

Handling Constraints

Several possible ways to handle constraints, e.g.:

- resampling until a new feasible point is found (“often bad idea”)
- penalty function approach: add constraint violation term (potentially scaled)
- repair approach: after generation of a new point, repair it (e.g. with a heuristic) to become feasible again if infeasible
  - continue to use repaired solution in the population or
  - use repaired solution only for the evaluation?
- multiobjective approach: keep objective function and constraint functions separate and try to optimize all of them in parallel
- ...

Examples for some EA parts

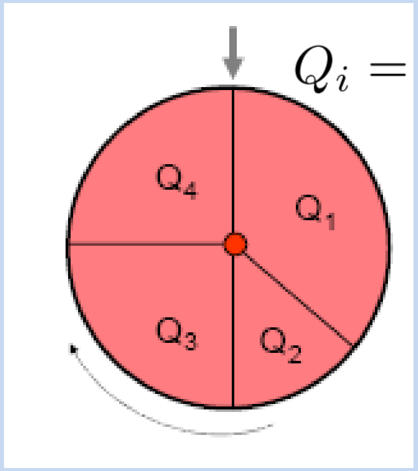
Selection

Selection is the major determinant for specifying the trade-off between exploitation and exploration

Selection is either

stochastic or deterministic

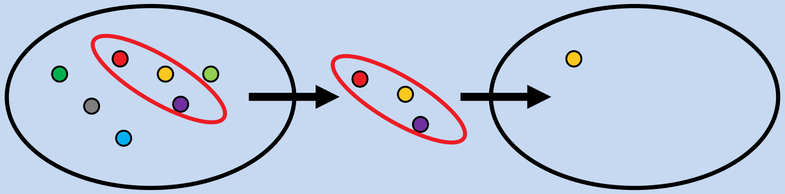
e.g. fitness proportional



$$Q_i = \frac{f(x_i)}{\sum_{j=1}^{\mu} f(x_j)}$$

Disadvantage: depends on scaling of f

e.g. via a tournament



e.g. $(\mu+\lambda)$, (μ,λ)

best μ from offspring *and* parents

best μ from offspring only

Mating selection (selection for variation): usually stochastic

Environmental selection (selection for survival): often deterministic

Variation Operators

Variation aims at generating new individuals on the basis of those individuals selected for mating

Variation = Mutation and Recombination/Crossover

mutation: *mut:* $\Omega \rightarrow \Omega$

recombination: *recomb:* $\Omega^r \rightarrow \Omega^s$ where $r \geq 2$ and $s \geq 1$

- choice always depends on the problem and the chosen representation
- however, there are some operators that are applicable to a wide range of problems and tailored to standard representations such as vectors, permutations, trees, etc.

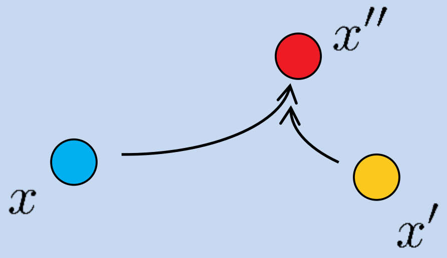
Variation Operators: Guidelines

Two desirable properties for mutation operators:

- every solution can be generation from every other with a probability greater than 0 (“exhaustiveness”)
- $d(x,x') < d(x,x'') => Prob(\mathrm{mut}(x) = x') > Prob(\mathrm{mut}(x) = x'')$ (“locality”)

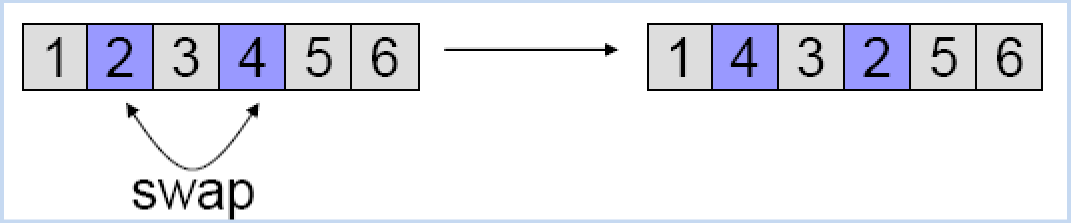
Desirable property of recombination operators (“in-between-ness”):

$$x'' = \ \mathrm{recomb}(x,x') \Rightarrow d(x'',x) \leq d(x,x') \wedge d(x'',x') \leq d(x,x')$$

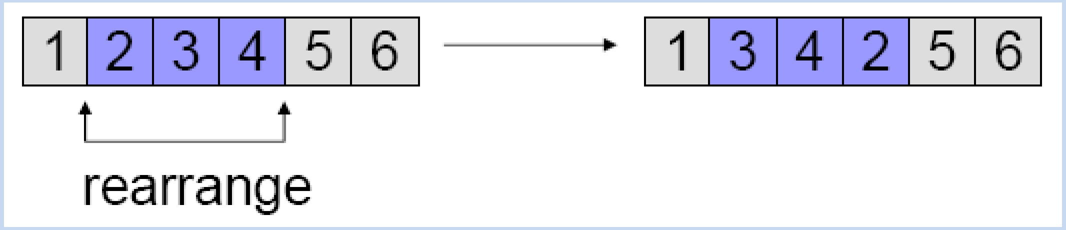


Examples of Mutation Operators on Permutations

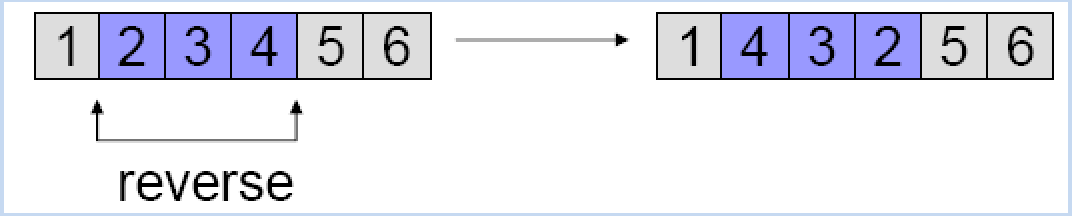
Swap:



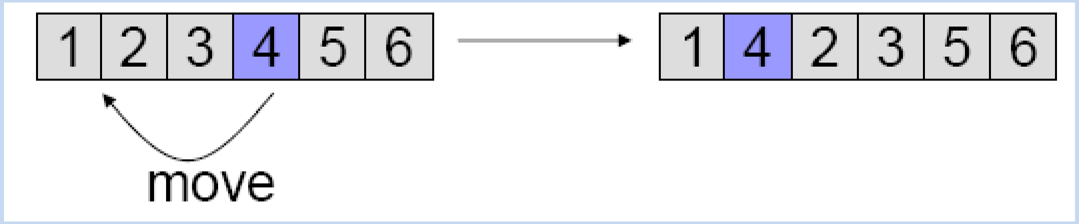
Scramble:



Invert:

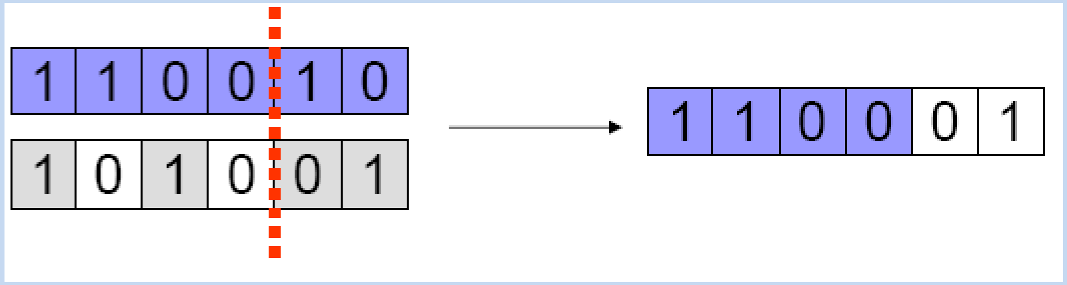


Insert:

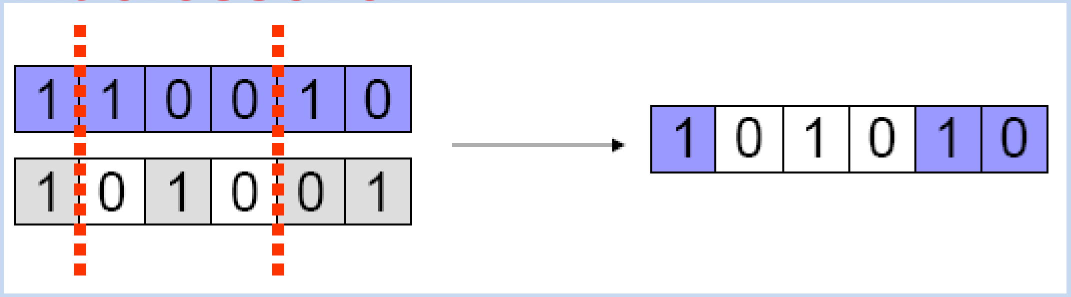


Examples of Recombination Operators: $\{0,1\}^n$

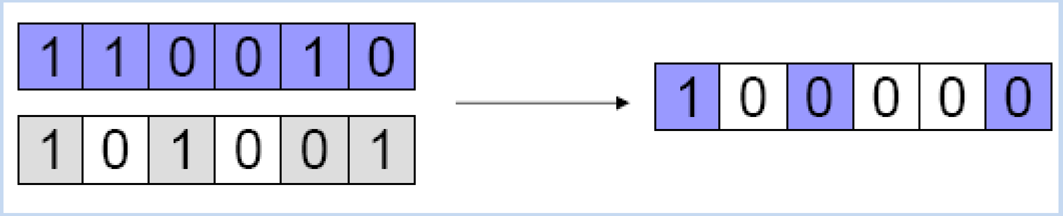
1-point crossover



n-point crossover



uniform crossover



choose each bit independently from one parent or another

A Canonical Genetic Algorithm

- binary search space, maximization
- uniform initialization
- generational cycle: of the population
  - evaluation of solutions
  - mating selection (e.g. roulette wheel)
  - crossover (e.g. 1-point)
  - environmental selection (e.g. plus-selection)

Conclusions

- EAs are generic algorithms (randomized search heuristics, meta-heuristics, ...) for black box optimization

  no or almost no assumptions on the objective function

- They are typically less efficient than problem-specific (exact) algorithms (in terms of #funevals)

  less differences in the continuous case (as we have seen)

- Allow for an easy and rapid implementation and therefore to find good solutions fast

  easy to incorporate (and recommended!) to incorporate problem-specific knowledge to improve the algorithm

Conclusions

I hope it became clear...

...that heuristics is what we typically can afford in practice (no guarantees and no proofs)

...what are the main ideas behind evolutionary algorithms

...and that evolutionary algorithms and genetic algorithms are no synonyms