Introduction to Optimization

Lecture 2: Dynamic Programming and Branch&Bound

September 25, 2015

TC2 - Optimisation

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supplementary material to last week's lecture

Prim's Algorithm for Minimum Spanning Trees

Remember:

- construct MST by adding the node (greedily) which connects to the current tree and has minimal weight (without introducing a cycle)

Question was:

- isn't the runtime better than for Kruskal's algorithm?
- reasoning was: we have to do "less global" things here

Answer:

- Kruskal: $O(|E| \log |E|)$ with simple data structures
- Prim: $O(|E| + |V| \log |V|)$ with Fibonacci heap and adjacency lists
  - this is linear in $|E|$ if $|E|$ is large enough (if $|E| = \Omega(|V| \log |V|)$)
  - but also Kruskal can be made almost linear by using the union-by-size heuristic and path compression (amortized time $O(|E| \log^* |V|)$)

  $\log^* n = \min \{s \mid \underbrace{\log(\log(\ldots \log(n) \ldots))}_{s \text{ times}} \leq 1\}$

Announcements

Mid-term Exam (aka “contrôle continu”)

- we will have *two* larger home exercises
- 1st hand-out ready by today (discrete part, already online)
- to be solved at home in addition to the lecture
- hand-in by e-mail until **Friday, October 16 (beginning of lecture)**
- second home exercise available soon (continuous part)
- both are graded together: need 50% of points to pass, counts as 1/3 of overall grade

All information also available at

`http://researchers.lille.inria.fr/~brockhof/optimizationSaclay/`

(exercise sheets, lecture slides, additional information, links, ...)

Presentation Blackbox Optimization Lecture

Presentation Black Box Optimization Lecture

- Optional class “Black Box Optimization”
- Taught also by Anne Auger and me
- Advanced class, (even) closer to our actual research topic

Goals:

❶ present the latest knowledge on blackbox optimization algorithms and their foundations

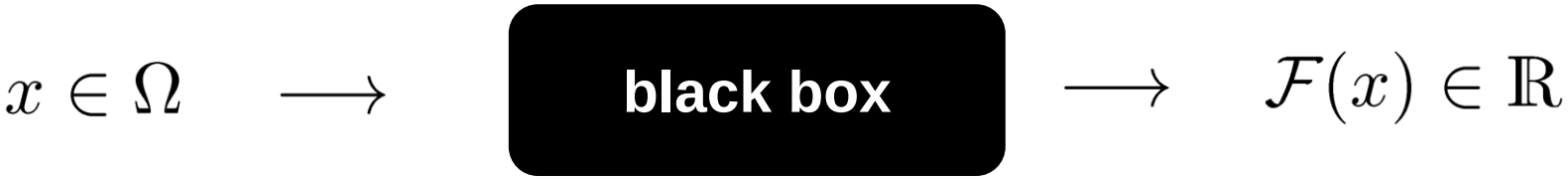
❷ offer hands-on exercises on difficult common optimization problems

❸ give insights into what are current challenging research questions in the field of blackbox optimization (as preparation for a potential Master’s or PhD thesis in the field)

☺ relatively young research field with many interesting research questions (in both theory and algorithm design)

☺ related to real-world problems: also good for a job outside academia

Black Box Scenario



Why are we interested in a black box scenario?

- objective function F often noisy, non-differentiable, or sometimes not even understood or available
- objective function F contains lecagy or binary code, is based on numerical simulations or real-life experiments
- most likely, you will see such problems in practice...

Objective: find x with small F(x) with as few function evaluations as possible

assumption: internal calculations of algo irrelevant

What Makes an Optimization Problem Difficult?

- Search space too large

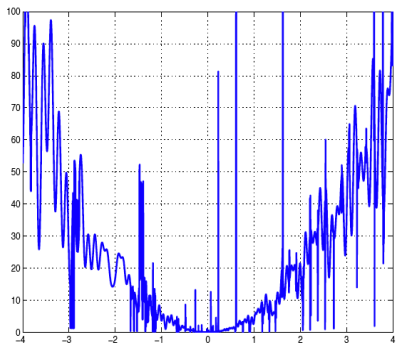
  exhaustive search impossible

- Non conventional objective function or search space

  mixed space, function that cannot be computed

- Complex objective function

  non-smooth, non differentiable, noisy, ...



stochastic search algorithms
well suited because they:

- don't make many assumptions on f
- are invariant wrt. translation/rotation of the search space, scaling of f, ...
- are robust to noise

Planned Topics / Keywords

- Introduction to stochastic search algorithms, in particular
  - Evolutionary algorithms
  - Evolution Strategies and the CMA-ES algorithm
  - Algorithms for large-scale problems (“big data”)
- Benchmarking black box algorithms
- Multiobjective optimization

- Again: combination of lectures & exercises, theory & practice
- Connections with machine learning class of M. Sebag

Course Overview

Date		Topic
Fri, 18.9.2015	DB	Introduction and Greedy Algorithms
Fri, 25.9.2015	DB	Dynamic programming and Branch and Bound
Fri, 2.10.2015	DB	Approximation Algorithms and Heuristics
Fri, 9.10.2015	AA	Introduction to Continuous Optimization
Fri, 16.10.2015	AA	End of Intro to Cont. Opt. + Gradient-Based Algorithms I
Fri, 30.10.2015	AA	Gradient-Based Algorithms II
Fri, 6.11.2015	AA	Stochastic Algorithms and Derivative-free Optimization
16 - 20.11.2015		Exam (exact date to be confirmed)

all classes + exam are from 14h till 17h15 (incl. a 15min break)
here in PUIO-D101/D103

Overview of Today's Lecture

Dynamic Programming

- shortest path problem
  - Dijkstra's algorithm
  - Floyd's algorithm
- exercise: a dynamic programming algorithm for the knapsack problem (KP)

Branch and Bound

- applied to Integer Linear Programs

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

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:

1. decompose the problem into subproblems and think about how to solve a larger problem with the solutions of its subproblems
2. specify how you compute the value of a larger problem recursively with the help of the optimal values of its subproblems ("Bellman equation")
3. bottom-up solving of the subproblems (i.e. computing their optimal value), starting from the smallest by using a table structure to store the optimal values and the Bellman equality

   (top-down approach also possible, but less common)
4. eventually construct the final solution (can be omitted if only the value of an optimal solution is sought)

Bellman Equation (aka “Principle of Optimality”)

- introduced by R. Bellman as “Principle of Optimality” in 1957
- the basic equation underlying dynamic programming
- necessary condition for optimality

citing Wikipedia:

> “Richard Bellman showed that a dynamic optimization problem in discrete time can be stated in a recursive, step-by-step form known as backward induction by writing down the relationship between the value function in one period and the value function in the next period. The relationship between these two value functions is called the "Bellman equation".”
>
> - The value function here is the objective function.
> - The Bellman equation exactly formalizes how to compute the optimal function value for a larger subproblem from the optimal function value of smaller subproblems.

we will see examples later today...

Historical Note

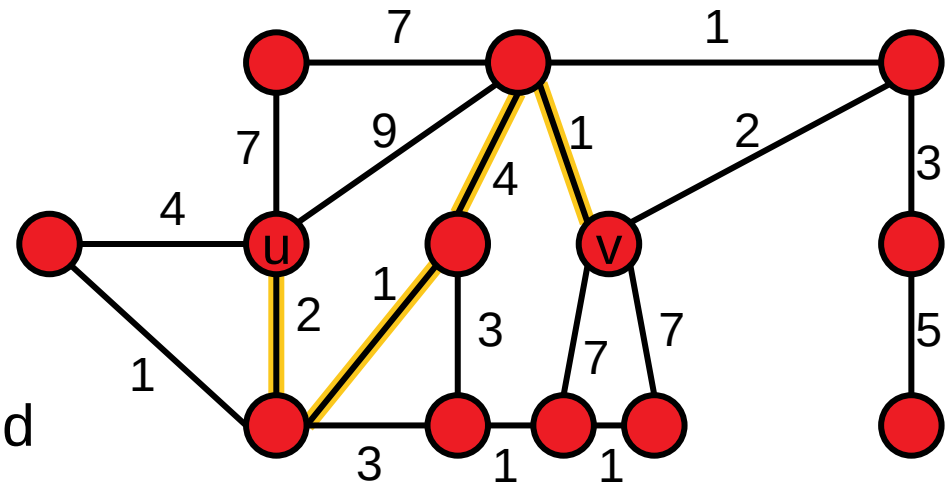
Why is it called “dynamic” and why “programming”?

- R. Bellman worked at the time, when he “invented” the idea, at the RAND Corporation who were strongly connected with the Air Force
- In order to avoid conflicts with the head of the Air Force at this time, R. Bellman decided against using terms like “mathematical” and he liked the word *dynamic* because it “has an absolutely precise meaning” and cannot be used “in a pejorative sense”
- in addition, it had the right meaning: “I wanted to get across the idea that this was dynamic, this was multistage, this was time-varying.”
- Citing Wikipedia: “The word *programming* referred to the use of the method to find an optimal *program*, in the sense of a military schedule for training or logistics.”

Reminder: 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.



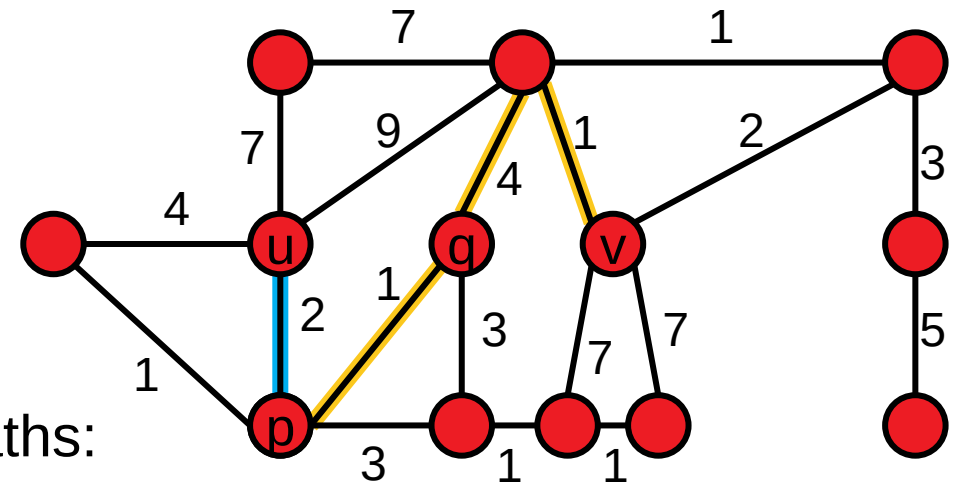
Note:

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

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 Algorithm of E. Dijkstra (1956)

ShortestPathDijkstra(G, D, source, target):

Initialization:

- dist(source) = 0 and for all $v \in V$: dist(v)= ∞
- for all $v \in V$: prev(v) = null # predecessors on opt. path
- U = V # U: unexplored vertices

Unless U empty or target visited do:

- newNode = $\text{argmin}_{u \in U} \{\text{dist}(u)\}$
- remove newNode from U
- for each neighbor v of newNode do:
  - altDist = dist(newNode) + $D_{\text{newNode},v}$
  - if altDist < dist(v):
    - dist(v) = altDist
    - prev(v) = u

Very Short Exercise

Question:

Is Dijkstra's algorithm a dynamic programming algorithm?

Answer:

- that is a tricky question ;-)
- it has greedy elements, but also stores the answers to subproblems without recomputing them
- so, actually, it is a dynamic programming algorithm with a greedy selection of the next subproblem to be computed

The Algorithm of R. Floyd (1962)

Idea:

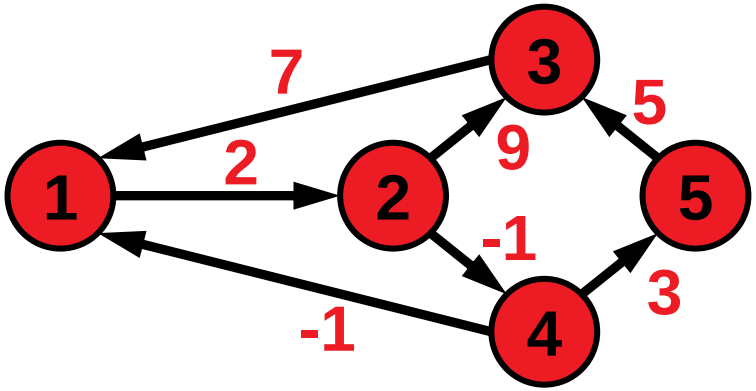
- if we knew that the shortest path between source and target goes through node v, we would be able to construct the optimal path from the shorter paths "source→v" and "v→target"
- subproblem P(k): compute all shortest paths where the intermediate nodes can be chosen from v_1, ..., v_k

ShortestPathFloyd(G, D, source, target) [= AllPairsShortestPath(G)]

- 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. $1 \leq i,j \leq |V|$):
    - $dist(i,j) = \min \{ dist(i,j), dist(i,k) + dist(k,j) \}$

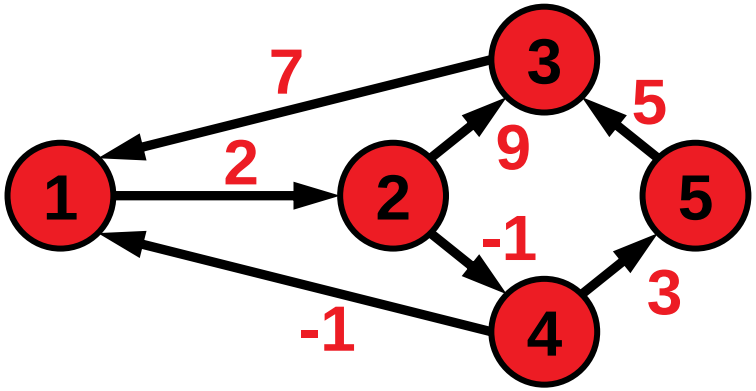
Note: This algorithm has the advantage that it can handle negative weights as long as no cycle with negative total weight exists

Example



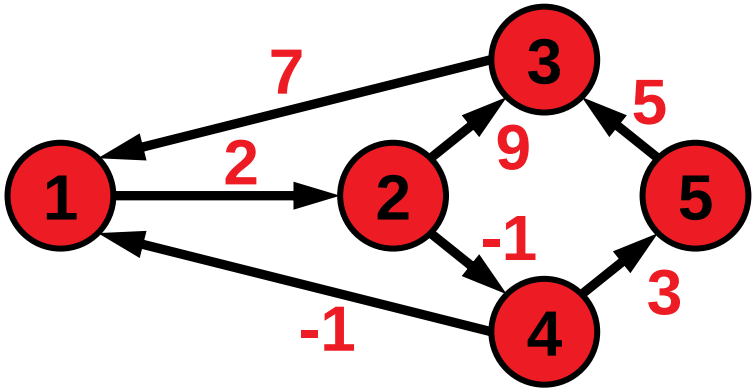
k=0	1	2	3	4	5
1					
2					
3					
4					
5					

Example



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

Example

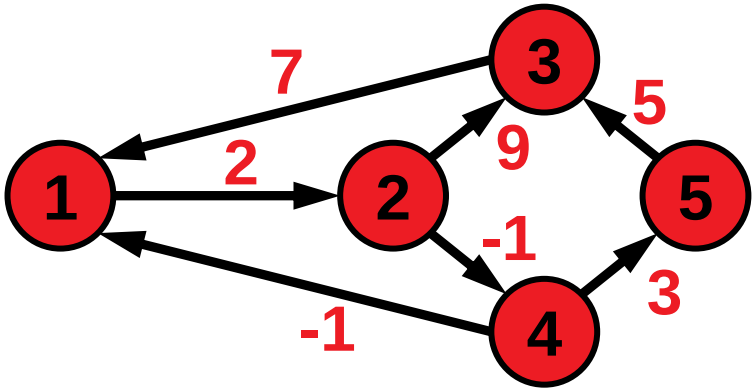


allow 1 as intermediate node

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					
2					
3					
4					
5					

Example



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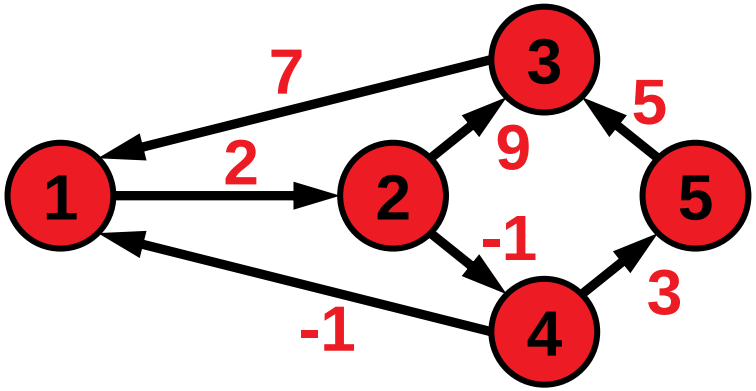
3	7	∞	∞	∞	∞
4	1	∞	∞	∞	3
5	∞	∞	5	∞	∞

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

Example



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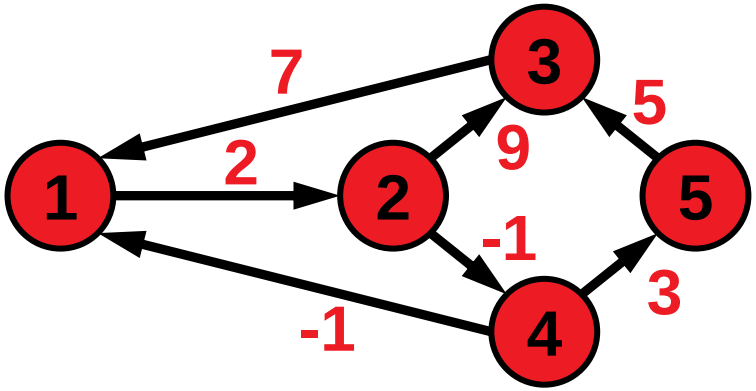
3	7	∞	∞	∞	∞
4	1	∞	∞	∞	3
5	∞	∞	5	∞	∞

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

Example



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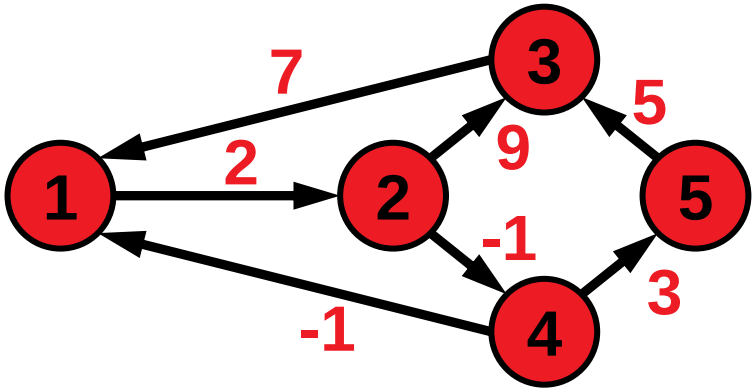
2	∞	∞	9	-1	∞
3	7	∞	∞	∞	∞
4	1	∞	∞	∞	3
5	∞	∞	5	∞	∞

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

Example



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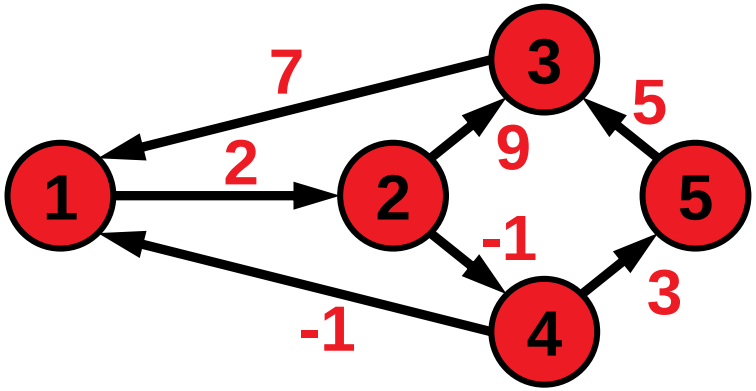
k=0	1	2	3	4	5
1	∞	2	∞	∞	∞
2	∞	∞	9	-1	∞
3	7	∞	∞	∞	∞
4	1	∞	∞	∞	3
5	∞	∞	5	∞	∞

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

Example

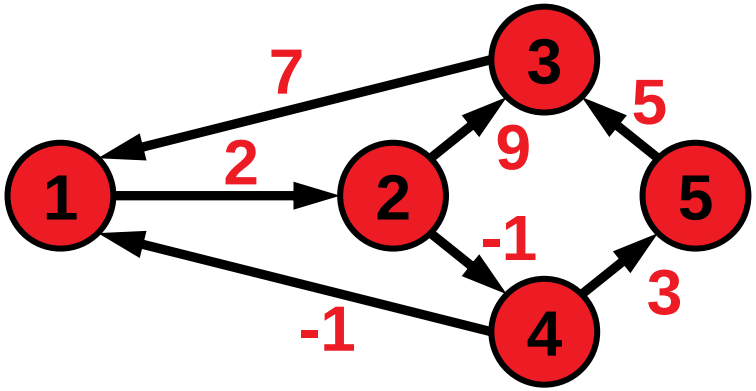


allow 1 & 2 as intermediate nodes

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



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	∞	∞

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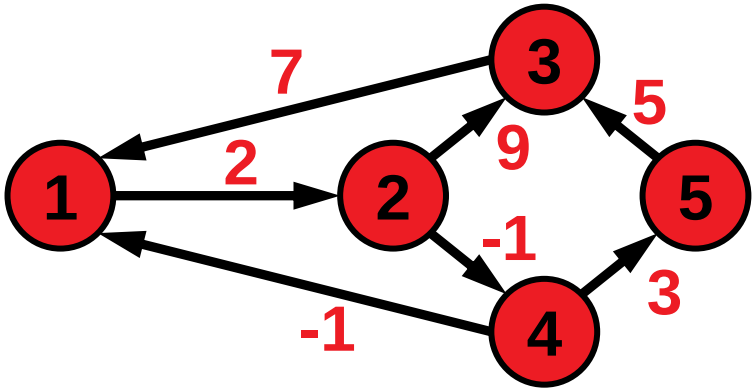

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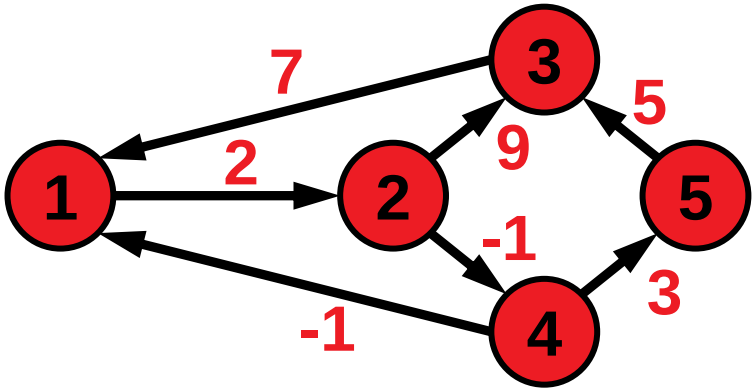
2	∞	∞	9	-1	∞
3	7	9	∞	∞	∞
4	-1	1	∞	∞	3
5	∞	∞	5	∞	∞

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

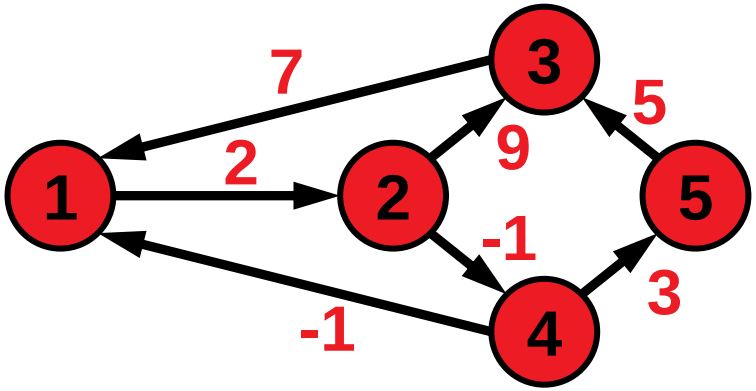


allow {1,2,3} as intermediate nodes

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



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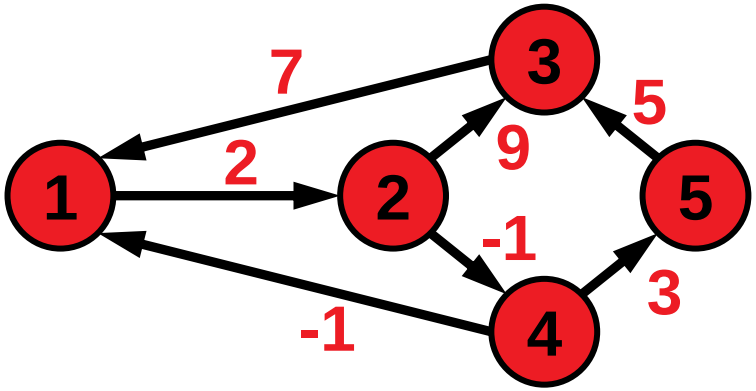
5	∞	∞	5	∞	∞

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

Example



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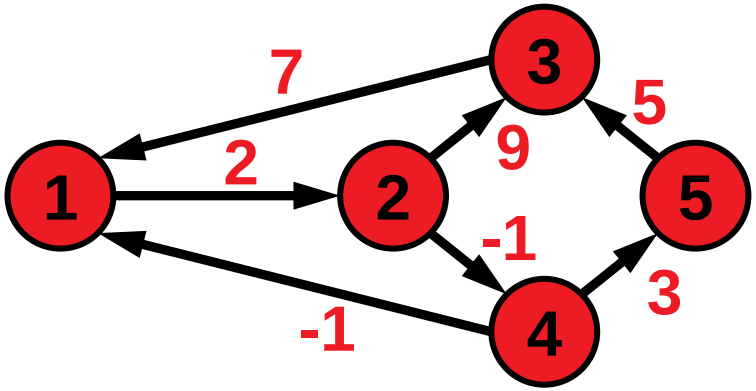
4	-1	1	10	0	3
5	∞	∞	5	∞	∞

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

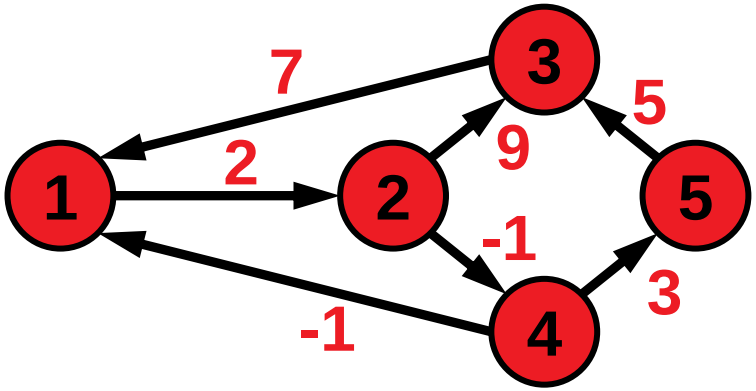


allow {1,2,3,4} as intermediate nodes

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



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

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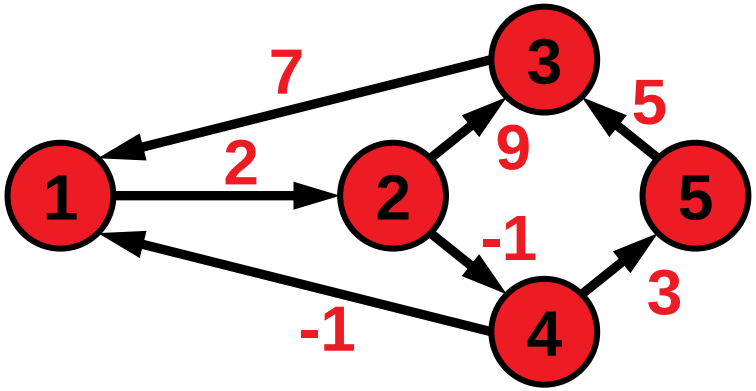
2	16	18	9	-1	∞
3	7	9	18	8	∞
4	-1	1	10	0	3
5	12	14	5	13	∞

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

Example

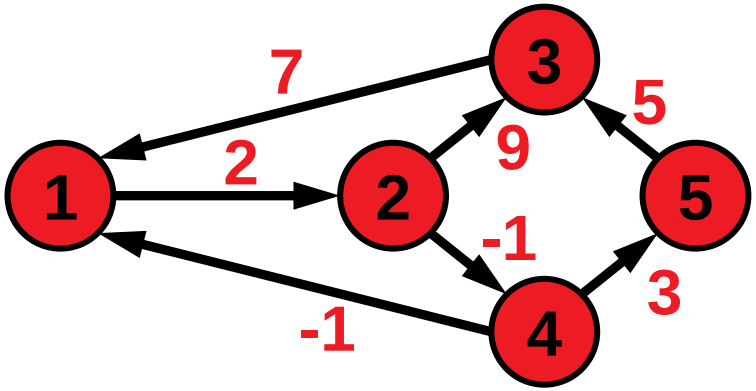


allow {1,2,3,4} as intermediate nodes

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

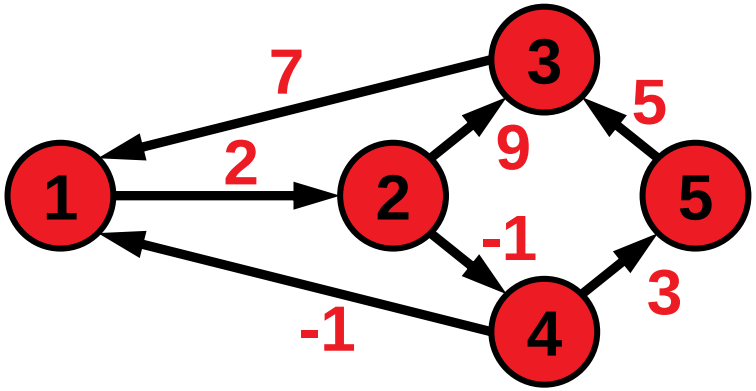


allow all nodes as intermediate nodes

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



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4	-1	1	8	0	3
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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
- $P_{i,j}$ = predecessor of node j on path from i to j
- no extra costs (asymptotically)

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

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

Exercise:
The Knapsack Problem and Dynamic Programming

http://researchers.lille.inria.fr/~brockhof/optimizationSaclay/

Branch and Bound

Branch and Bound: General Ideas

- Systematic enumeration of candidate solutions in terms of a rooted tree
- Each tree node corresponds to a set of solutions; the whole search space on the root
- At each tree node, the corresponding subset of the search space is split into (non-overlapping) sub-subsets:
  - the optimum of the larger problem must be contained in at least one of the subproblems
- If tree nodes correspond to small enough subproblems, they are solved exhaustively.
- The smart part of the algorithm is the estimation of upper and lower bounds on the optimal function value achieved by solutions in the tree nodes
  - the exploration of a tree node is stopped if a node's upper bound is already lower than the lower bound of an already explored node (assuming maximization)

Applying Branch and Bound

Needed for successful application of branch and bound:

- optimization problem
- finite set of solutions
- clear idea of how to split problem into smaller subproblems
- efficient calculation of the following modules:
  - upper bound calculation
  - lower bound calculation

Computing Bounds (Maximization Problems)

Assume w.l.o.g. maximization of f(x) here

Lower Bounds

- any actual feasible solution will give a lower bound (which will be exact if the solution is the optimal one for the subproblem)
- hence, sampling a (feasible) solution can be one strategy
- using a heuristic to solve the subproblem another one

Upper Bounds

- upper bounds can be achieved by solving a relaxed version of the problem formulations (i.e. by either loosening or removing constraints)

Note: the better/tighter the bounds, the quicker the branch and bound tree can be pruned

Properties of Branch and Bound Algorithms

- Exact, global solver
- Can be slow; only exponential worst-case runtime
  - due to the exhaustive search behavior if no pruning of the search tree is possible
- but might work well in some cases

Advantages:

- can be stopped if lower and upper bound are “close enough” in practice (not necessarily exact anymore then)
- can be combined with other techniques, e.g. “branch and cut” (not covered here)

Example Branching Decisions

0-1 problems:

- choose unfixed variable x_i
- one subproblem defined by setting x_i to 0
- one subproblem defined by setting x_i to 1

General integer problem:

- choose unfixed variable x_i
- choose a value c that x_i can take
- one subproblem defined by restricting $x_i \leq c$
- one subproblem defined by restricting $x_i > c$

Combinatorial Problems:

- branching on certain discrete choices, e.g. an edge/vertex is chosen or not chosen

The branching decisions are then induced as additional constraints when defining the subproblems.

Which Tree Node to Branch on?

Several strategies (again assuming maximization):

- choose the subproblem with highest upper bound
  - gain the most in reducing overall upper bound
  - if upper bound not the optimal value, this problem needs to be branched upon anyway sooner or later
- choose the subproblem with lowest lower bound
- simple DFS or BFS
- problem-specific approach most likely to be a good choice

4 Steps Towards a Branch and Bound Algorithm

Concrete steps when designing a branch and bound algorithm:

- How to split a problem into subproblems ("branching")?
- How to compute upper bounds (assuming maximization)?
- Optional: how to compute lower bounds?
- How to decide which next tree node to split?

now: example of integer linear programming
mid-term exam: application to knapsack problem

Application to ILPs

$$\begin{aligned} \text{maximize} \quad & c^T x \\ \text{subject to} \quad & Ax \leq b \\ & x \geq 0 \\ \text{and} \quad & x \in \mathbb{Z}^n \end{aligned}$$

The ILP formalization covers many problems such as

- Traveling Salesperson Person (TSP)
- Vertex Cover and other covering problems
- Set packing and other packing problems
- Boolean satisfiability (SAT)

Ways of Solving an ILP

- Do not restrict the solutions to integers and round the solution found of the relaxed problem (=remove the integer constraints) by a continuous solver (i.e. solving the so-called *LP relaxation*)

  → no guarantee to be exact
- Exploiting the instance property of A being total unimodular:
  - feasible solutions are guaranteed to be integer in this case
  - algorithms for continuous relaxation can be used (e.g. the simplex algorithm)
- Using heuristic methods (typically without any quality guarantee)
  - we'll see these type of algorithms in next week's lecture
- Using exact algorithms such as branch and bound

Branch and Bound for ILPs

Here, we just give an idea instead of a concrete algorithm...

- How to split a problem into subproblems (“branching”)?
- How to compute upper bounds (assuming maximization)?
- Optional: how to compute lower bounds?
- How to decide which next tree node to split?

Branch and Bound for ILPs

Here, we just give an idea instead of a concrete algorithm...

- How to compute upper bounds (assuming maximization)?
- How to split a problem into subproblems (“branching”)?
- Optional: how to compute lower bounds?
- How to decide which next tree node to split?

Branch and Bound for ILPs

How to compute upper bounds (assuming maximization)?

- drop the integer constraints and solve the so-called LP-relaxation
- can be done by standard LP algorithms such as `scipy.optimize.linprog` or Matlab's `linprog`

What's then?

- The LP has no feasible solution. Fine. Prune.
- We found an integer solution. Fine as well. Might give us a new lower bound to the overall problem.
- The LP problem has an optimal solution which is worse than the highest lower bound over all already explored subproblems. Fine. Prune.
- Otherwise: Branch on this subproblem: e.g. if optimal solution has $x_i=2.7865$, use $x_i \leq 2$ and $x_i \geq 3$ as new constraints

Branch and Bound for ILPs

How to split a problem into subproblems ("branching")?

- mainly needed if the solution of the LP-relaxation is not integer
- branch on a variable which is rational

Not discussed here in depth due to time:

- Optional: how to compute lower bounds?
- How to decide which next tree node to split?
  - seems to be good choice: subproblem with largest upper bound of LP-relaxation

Conclusions

I hope it became clear...

...what the algorithm design ideas of dynamic programming and branch and bound are

...for which problem types they are supposed to be suitable

...and how to apply the dynamic programming idea to the knapsack problem