Heuristic Algorithms for Combinatorial Optimization problems

Ph.D. course in Computer Science

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Aims of the course

This course aims to

1. show that heuristic algorithms are not recipes for specific problems: heuristics and problems can be matched freely
   (*of course, with different performance*)
2. discuss the common and general aspects of these algorithms
3. teach how to design a heuristic for a specific problem
4. teach how to evaluate its performance

Heuristics

eurisko = I find

It is a word derived from Greek

- inspired by the famous story of Archimedes and the golden crown

but it was

- never used by the ancient Greeks
- coined during the 19th century

Some historical facts

- 4th century CE: Pappus of Alexandria discusses the *analyòmenos* (*treasure of analysis*), that is how to build a mathematical proof
  - how to move from the hypotheses to the thesis of a theorem
  - how to move from the data to the solution of a geometrical problem
- 17th century: Descartes, Leibnitz *et al.* discuss the ars inveniendi (*art of finding*), *i. e.* the attainment of truth through mathematics
- 19th century: Bernard Bolzano discusses in detail the most common strategies to build mathematical proofs (*Erfindungskunst*)
- 19th-20th century: phylosophers, psychologists and economists define heuristics as practical and simple decision rules that do not aim at an optimal result, but at a satisficing one (Simon, 1957)
- 1945: the short essay *How to solve it* by György Pólya comes back to the mathematical meaning of heuristic as an informal process that leads to prove a thesis or to find a solution

So, what about *heuristic algorithms*?

Algorithms and heuristics

Some scientific sectors use the two words as opposites:

- algorithm as a formal, deterministic procedure, consisting of a finite sequence of elementary steps
- heuristic as an informal, creative, open rule

One could even say that

- an algorithm is a correctness proof
- a heuristic is a bunch of common sense arguments

In fact, an algorithm has a correctness proof, a heuristic has none

The phrase heuristic algorithm is an oxymoron, in some respects

Then what does it mean?

Heuristic algorithms

A heuristic algorithm is an algorithm which does not guarantee a correct solution

Then it is useless!

Quite to the contrary, it can be useful, provided that

1. it "costs" much less than a correct algorithm:
   this requires a definition of computational cost of an algorithm
   - time
   - space
2. it "frequently" yields something "close" to the correct solution:
   this requires to define a solution space endowed with
   - a metric to express a "satisfactory distance" from the correct solution
   - a probabilistic distribution to express the "satisfactory frequence" of solutions at a satisfactory distance from the correct solutions

Proofs and algorithms

Mathematical proofs and algorithms are strictly related

- every algorithm has/is a correctness proof
- both are mechanical symbolic transformations from a starting point (hypotheses/data) to an ending point (thesis/solution)
- Turing's undecidability proof mirrors Gödel's incompleteness proof

Heuristics are the construction of both proofs and algorithms

- in case of success, the heuristic is abandoned and the proof preserved
- otherwise, a good heuristic frequently provides a good result, instead of always providing a perfect one

This is the motivation for heuristic algorithms

The focus of this course

The course focuses on heuristic algorithms

- that apply to Combinatorial Optimization problems
- that are solution-based (as opposed to model-based)

So, we limit

1. the kind of problem
2. the kind of algorithm

It is still a pretty wide field

Let us further discuss the two limitations

Problem classification

A problem is a question on a mathematical system

Problems can be classified based on the nature of their solution:

- decision problems: their solution is either *True* or *False*
- search problems: their solution is any feasible subsystem (that is, satisfying certain conditions)
- optimization problems: their solution is the minimum or maximum value of an objective function defined on the feasible subsystems
- counting problems: their solution is the number of feasible subsystems
- enumeration problem: their solution is the collection of all feasible subsystems
- ...

We address the combination of optimization and search, that is, we look for the optimal value and a subsystem assuming that value

Optimization/search problems

An optimization/search problem can be represented as

$$\begin{array}{l} \text{opt } f(x) \\ x \in X \end{array}$$

where

- a solution x describes each subsystem of the problem
- the feasible region X (feasible solution space) is the set of subsystems which satisfy given conditions
- the objective function $f : X \to \mathbb{R}$ quantitatively measures the quality of each subsystem ($\text{opt} \in \{\min, \max\}$)

The problem consists in determining

- optimization: the optimal value f^* of the objective function:

$$f^* = \underset{x \in X}{\text{opt}}\, f(x)$$

- search: at least one optimal solution, that is a subsystem

$$x^* \in X^* = \arg \underset{x \in X}{\text{opt}}\, f(x) = \left\{ x^* \in X : f(x^*) = \underset{x \in X}{\text{opt}}\, f(x) \right\}$$

Why focusing on optimization/search problem?

- applications: objects with extreme values of an evaluation function tend to be very useful
  - low energy protein structures
  - highly influential/influentiable groups of individuals in social networks
  - low violation partitions of points into regular shapes (classifications)
  - small expressions of logical functions
  - ...

  Exact optimality is costly, not always required, or even desirable (*many heuristic solutions could be preferable to a single exact one*)
- hard decision/search problems reduce to optimization/search by relaxing the complicating constraints
  - enlarge the feasible region from X to $X' \supset X$ to make the search easy;
  - quantify the distance $d(x)$ of every $x \in X'$ from X;
  - minimize $d(x)$ in X': $d(x^*) = 0 \Leftrightarrow x^* \in X$
- enumeration problems of Paretian frontiers (compromises among conflicting objectives) directly adapt optimization/search algorithms

Combinatorial Optimization (*CO*)

A problem is a *CO* problem when the feasible region X is a finite set, that is, it has a finite number of feasible solutions

This looks like a very restrictive assumption

However, the study of *CO* problems can be useful more in general:

1. infinite discrete problems can have a finite set of interesting solutions
2. some continuous problems can be reduced to *CO* problems
   (*e. g., Linear Programming, Maximum Flow, Minimum Cost Flow*)
3. continuous problems can be reduced to discrete ones by sampling
   (*usually not very effective*)
4. ideas conceived for *CO* problems can be extended to other problems
   (*often quite effective*)

Model-based heuristics

They describe the feasible region X with a "model"

A typical example is a Mathematical Programming formulation

$$\begin{array}{l} \text{opt } f(x) \\ x \in X \end{array} \longrightarrow \begin{array}{ll} \text{min } \phi(\xi) & \\ g_i(\xi) \leq 0 & i = 1, \ldots, m \end{array}$$

where

- $\xi \in \mathbb{R}^n$, that is, a solution is a vector of n real values
- $X = \{\xi \in \mathbb{R}^n : g_i(\xi) \leq 0, i = 1, \ldots, m\}$, that is, the feasible region is the set of vectors which satisfy all the inequalities (constraints)

Model-based heuristics exploit the information derived from the model, that is the analytical properties of functions ϕ and g_i $(i = 1, \ldots, m)$

Other models can be based on *SAT*, etc...

We will not use these tools

An alternative definition of *CO*

A problem is a *CO* problem when:

1. the number of feasible solutions is finite
2. the feasible region is $X \subseteq 2^B$ for a given finite ground set B, that is, the feasible solutions are all subsets of the ground set that satisfy suitable conditions

The two definitions are equivalent:

$2 \Rightarrow 1$: if the ground set B is finite, every collection $X \subseteq 2^B$ is finite

$1 \Rightarrow 2$: if the number of feasible solutions is finite, define B as their set and the feasible region X as the collection of all singletons of B
(*a "solution" is a set containing a single solution*)

In general, the sophisticated definition allows a deeper analysis, because

- X is not simply enumerated
- X is defined in a compact and significant way

Solution-based heuristics: a classification for *CO* problems

Solution-based heuristics consider solutions as subsets of the ground set

1. constructive/destructive heuristics:
   - they start from an extremely simple subset (respectively, $\emptyset$ or B)
   - they add/remove elements until they obtain the desired solution
2. exchange heuristics:
   - they start from a subset obtained in any way
   - they exchange elements until they obtain the desired solution
3. recombination heuristics:
   - they start from a population of subsets obtained in any way
   - they recombine different subsets producing a new population

Heuristic designers can creatively combine elements from different classes

Randomization and memory

Two other distinctions concern

- the use of randomization:
  - deterministic heuristics, whose input includes only certain information
  - randomized heuristics, whose input includes pseudorandom numbers
    (*they are deterministic algorithms anyway*)
- the use of memory:
  - heuristics whose input includes only current information
  - heuristics whose input also includes previously generated solutions

These distinctions are independent from the previous classification

Metaheuristics (from the Greek, "beyond heuristics") is the common name for heuristic algorithms with randomization and/or memory

Risks to beware of

1. reverential or trendy attitude, that is choosing an algorithm based on the social context, instead of the problem
2. magic attitude, that is trusting a method on the basis of an analogy with physical and natural phenomena
3. heuristic integralism, that is using a heuristic for a problem which admits exact algorithms
4. number crunching, that is performing sophisticated and complex computations with unreliable numbers
5. SUV attitude, that is relying on hardware power
6. overcomplication, that is introducing redundant components and parameters, as if that could only improve the result
7. overfitting, that is adapting components and parameters of the algorithm to the specific dataset used in the experimental evaluation

It is fundamental to

- free oneself from prejudices
- evaluate the performance of the algorithm in a scientific way
- distinguish the contribution of each component of the algorithm
- efficiently implement each component of the algorithm

Combinatorial Optimization

$$\begin{array}{l} \text{opt } f(x) \\ x \in X \end{array}$$

where $X \subseteq 2^B$ and B finite

We will survey a number of problem classes

- set problems
- logic function problems
- numerical matrix problems
- graph problems

Why a problem survey?

Reviewing several problems is useful because

- abstract ideas must be concretely applied to different algorithms for different problems
- the same idea can have different effectiveness on different problems
- some ideas only work on problems with a specific structure
- different problems could have nonapparent relations, which could be exploited to design algorithms

So, a good knowledge of several problems teaches how to

- apply abstract ideas to new problems
- find and exploit relations between known and new problems

Sure, the "Magical Number Seven" risk exists...

To control it, we will make some interludes devoted to general remarks

Weighted set problems: Knapsack Problem (KP)

Given

- a set E of elementary objects
- a function $v : E \to \mathbb{N}$ describing the volume of each object
- a number $V \in \mathbb{N}$ describing the capacity of a knapsack
- a function $\phi : E \to \mathbb{N}$ describing the value of each object

select a subset of objects of maximum value that respects the capacity

The ground set is trivially the set of the objects: $B = E$

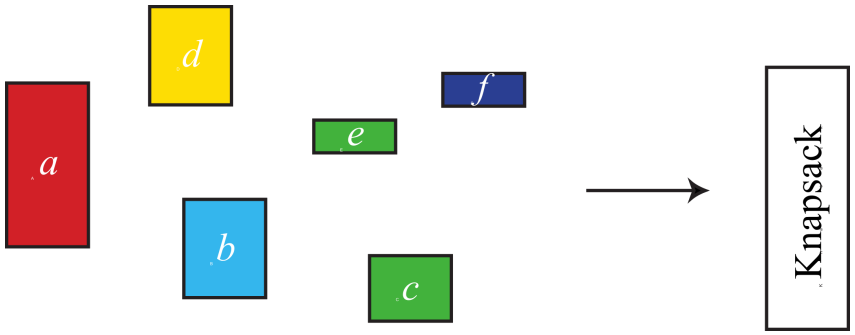
The feasible region includes all subsets of objects whose total volume does not exceed the capacity of the knapsack

$$X = \left\{ x \subseteq B : \sum_{j \in x} v_j \leq V \right\}$$

The objective is to maximize the total value of the chosen objects

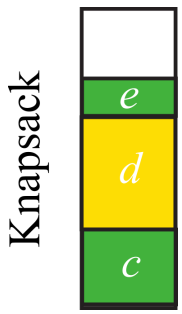
$$\max_{x \in X} f(x) = \sum_{j \in x} \phi_j$$

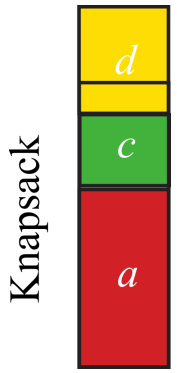
Example



E	a	b	c	d	e	f
ϕ	7	2	4	5	4	1
v	5	3	2	3	1	1

$V = 8$





$x' = \{c, d, e\} \in X$
$f(x') = 13$

$x'' = \{a, c, d\} \notin X$
$f(x'') = 16$

Set problems in metric spaces: *Maximum Diversity Problem (MDP)*

Given

- a set P of points
- a function $d : P \times P \to \mathbb{N}$ providing the distance between point pairs
- a number $k \in \{1, \ldots, |P|\}$ that is the number of points to select

select a subset of k points with the maximum total pairwise distance

The ground set is the set of points: $B = P$

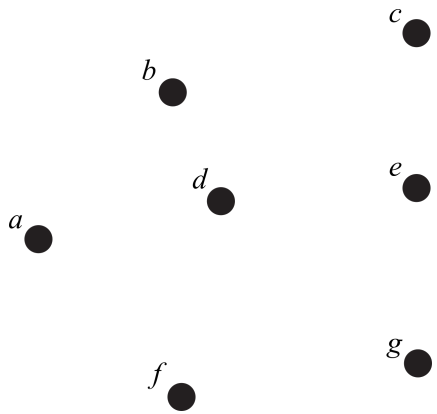
The feasible region includes all subsets of k points

$$X = \{x \subseteq B : |x| = k\}$$

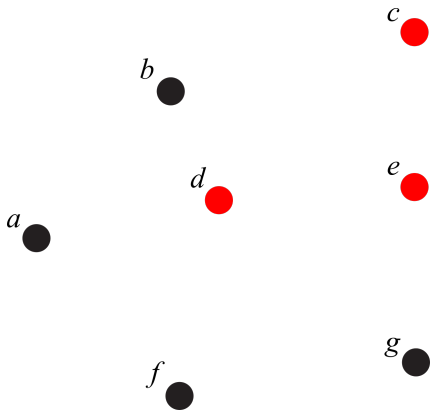
The objective is to maximize the sum of all pairwise distances between the selected points

$$\max_{x \in X} f(x) = \sum_{(i,j):i,j \in x} d_{ij}$$

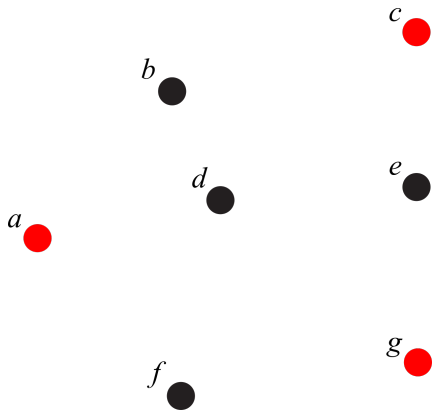
Example



$k = 3$



$x' = \{C, D, E\} \in X$
$f(x') = 24$



$x'' = \{A, C, G\} \in X$
$f(x'') = 46$

Interlude 1: the objective function

The objective function associates integer values to feasible subsets

$$f : X \to \mathbb{N}$$

Computing the objective function can be complex (even exhaustive)

We have seen two simple cases

- the *KP* has an additive objective function which sums values of an auxiliary function defined on the ground set

$$\phi : B \to \mathbb{N} \text{ induces } f(x) = \sum_{j \in x} \phi_j : X \to \mathbb{N}$$

- the *MDP* has a quadratic objective function

Both are defined not only on X, but on the whole of 2^B (*is this useful?*)

Both are easy to compute, but the additive functions $f(x)$ are also fast to recompute if subset x changes slightly: it is enough to

- sum ϕ_j for each element j added to x
- subtract ϕ_j for each element j removed from x

For quadratic functions, this seems more complex (*we will talk about it*)

Partitioning set problems: *Bin Packing Problem (BPP)*

Given

- a set E of elementary objects
- a function $v : E \to \mathbb{N}$ describing the volume of each object
- a set C of containers
- a number $V \in \mathbb{N}$ that is the volume of the containers

divide the objects into the minimum number of containers respecting the capacity

The ground set $B = E \times C$ includes all (object,container) pairs

The feasible region includes all partitions of the objects among the containers not exceeding the capacity of any container

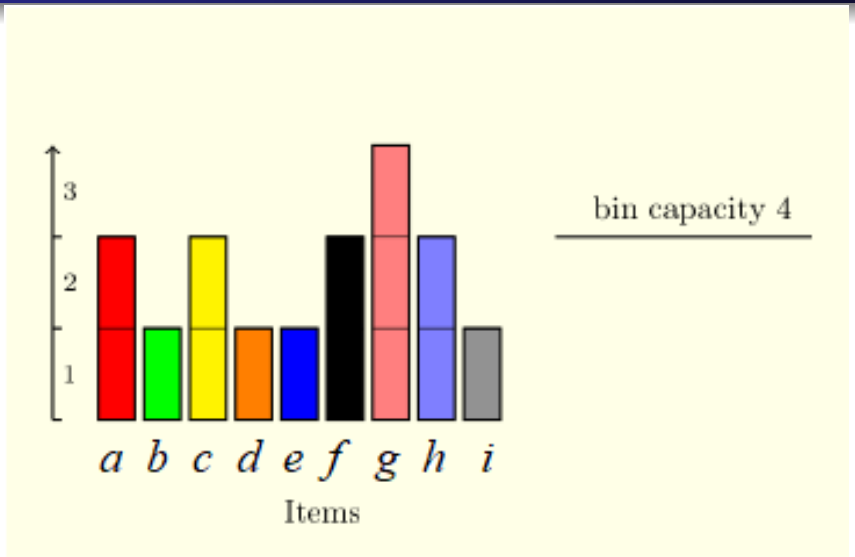
$$X = \left\{ x \subseteq B : |x \cap B_e| = 1 \; \forall e \in E, \sum_{(e,c) \in B^c} v_e \leq V \; \forall c \in C \right\}$$

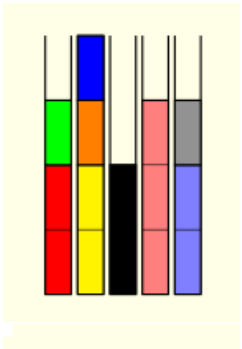
with $B_e = \{(i,j) \in B : i = e\}$ and $B^c = \{(i,j) \in B : j = c\}$

The objective is to minimize the number of containers used

$$\min_{x \in X} f(x) = |\{c \in C : x \cap B^c \neq \emptyset\}|$$

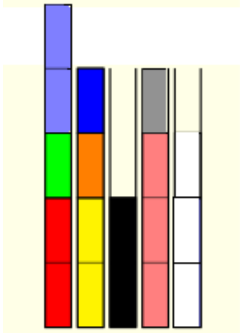
Example





$$x' = \{(a,1),(b,1),(c,2),(d,2),(e,2),(f,3),(g,4),(h,5),(i,5)\} \in X$$

$$f(x') = 5$$



$$x'' = \{(a,1),(b,1),(c,2),(d,2),(e,2),(f,3),(g,4),(h,1),(i,4)\} \notin X$$

$$f(x'') = 4$$

Partitioning set problems: *Parallel Machine Scheduling Problem (PMSP)*

Given

- a set T of tasks
- a function $d : T \to \mathbb{N}$ describing the time length of each task
- a set M of machines

divide the tasks among the machines with the minimum completion time

The ground set $B = T \times M$ includes all (task,machine) pairs

The feasible region includes all partitions of tasks among machines (*the order of the tasks is irrelevant!*)

$$X = \left\{ x \subseteq B : |x \cap B_t| = 1 \; \forall t \in T \right\}$$

The objective is to minimize the maximum sum of time lengths for each machine

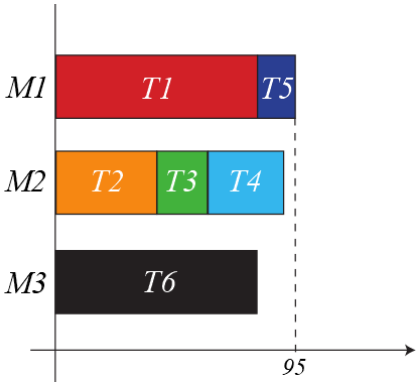
$$\min_{x \in X} f(x) = \max_{m \in M} \sum_{t:(t,m) \in x} d_t$$

Example

$$T = \{T1, T2, T3, T4, T5, T6\}$$

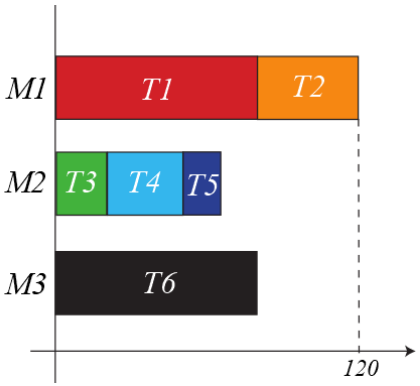
$$M = \{M1, M2, M3\}$$

task	$T1$	$T2$	$T3$	$T4$	$T5$	$T6$
d	80	40	20	30	15	80



$$x' = \{(T1, M1), (T2, M2), (T3, M2), (T4, M2), (T5, M1), (T6, M3)\} \in X$$

$$f(x') = 95$$



$$x'' = \{(T1, M1), (T2, M1), (T3, M2), (T4, M2), (T5, M2), (T6, M3)\} \in X$$

$$f(x'') = 120$$

Interlude 2: the objective function again

The objective function of the *BPP* and the *PMSP*

- is not additive
- is not trivial to compute (*but not hard, as well*)

Small changes in the solution have a variable impact on the objective

- equal to the time length of the moved tasks
  (e.g., move $T5$ on $M1$ in x'')
- zero (e.g., move $T5$ on $M3$ in x'')
- intermediate (e.g., move $T2$ on $M2$ in x'')

In fact, the impact of a change to the solution depends

- both on the modified elements
- and on the unmodified elements (*contrary to Interlude 1*)

The objective function is "flat": several solutions have the same value
(*this is a problem when comparing different modifications*)

Logic function problems: *Max-SAT* problem

Given a *CNF*, assign truth values to its logical variables so as to satisfy the maximum weight subset of its logical formulae

- a set V of logical variables x_j with values in $\mathbb{B} = \{0, 1\}$ (*false*, *true*)
- a literal ℓ_j is a function consisting of an affirmed or negated variable

$$\ell_j(x) \in \{x_j, \bar{x}_j\}$$

- a logical formula is a disjunction or logical sum (*OR*) of literals

$$C_i(x) = \ell_{i,1} \vee \ldots \vee \ell_{i,n_i}$$

- a conjunctive normal form (*CNF*) is a conjunction or logical product (*AND*) of logical formulae

$$CNF(x) = C_1 \wedge \ldots \wedge C_n$$

- to satisfy a logical function means to make it assume value 1
- a function w provides the weights of the *CNF* formulae

Logic function problems: *Max-SAT* problem

The ground set is the set of all simple truth assignments

$$B = V \times \mathbb{B} = \{(x_1, 0), (x_1, 1), \ldots, (x_n, 0), (x_n, 1)\}$$

The feasible region includes all subsets of simple assignments that are

- complete, that is include at least a literal for each variable
- consistent, that is include at most a literal for each variable

$$X = \{x \subseteq B : |x \cap B_v| = 1 \; \forall v \in V\}$$

with $B_{x_j} = \{(x_j, 0), (x_j, 1)\}$

The objective is to maximize the total weight of the satisfied formulae

$$\max_{x \in X} f(x) = \sum_{i : C_i(x) = 1} w_i$$

Example

- Variables
$$V = \{x_1, x_2, x_3, x_4\}$$
- Literals
$$L = \{x_1, \bar{x}_1, x_2, \bar{x}_2, x_3, \bar{x}_3, x_4, \bar{x}_4\}$$
- Logical formulae
$$C_1 = \bar{x}_1 \vee x_2 \qquad \ldots \qquad C_7 = x_2$$
- Conjunctive normal form

$$CNF = (\bar{x}_1 \vee x_2) \wedge (\bar{x}_1 \vee x_3) \wedge (\bar{x}_1 \vee \bar{x}_3) \wedge (\bar{x}_2 \vee x_4) \wedge (\bar{x}_2 \vee \bar{x}_4) \wedge x_1 \wedge x_2$$

- Weight function (uniform):
$$w_i = 1 \qquad i = 1, \ldots, 7$$

$x = \{(x_1, 0), (x_2, 0), (x_3, 1), (x_4, 1)\}$ satisfies $f(x) = 5$ formulae out of 7

Complementing a variable does not always change $f(x)$ (x_1 does, x_4 not)

Numerical matrix problems: Set Covering (*SCP*)

Given

- a binary matrix $A \in \mathbb{B}^{m,n}$ with row set R and column set C
- column $j \in C$ covers row $i \in R$ when $a_{ij} = 1$
- a function $c : C \to \mathbb{N}$ provides the cost of each column

Select a subset of columns covering all rows at minimum cost

The ground set is the set of columns: $B = C$

The feasible region includes all subsets of columns that cover all rows

$$X = \left\{ x \subseteq B : \sum_{j \in x} a_{ij} \geq 1 \; \forall i \in R \right\}$$

The objective is to minimize the total cost of the selected columns

$$\min_{x \in X} f(x) = \sum_{j \in x} c_j$$

Example

c	4	6	10	14	5	6

A						
	0	1	1	1	1	0
	0	0	1	1	0	0
	1	1	0	0	0	1
	0	0	0	1	1	1
	1	1	1	0	1	0

A							
	0	1	1	1	1	0	2
	0	0	1	1	0	0	1
	1	1	0	0	0	1	1
	0	0	0	1	1	1	1
	1	1	1	0	1	0	3

$$x' = \{c_1, c_3, c_5\} \in X$$

$$f(x') = 19$$

A							
	0	1	1	1	1	0	1
	0	0	1	1	0	0	0
	1	1	0	0	0	1	2
	0	0	0	1	1	1	2
	1	1	1	0	1	0	2

$$x'' = \{c_1, c_5, c_6\} \notin X$$

$$f(x'') = 15$$

"Set Covering": covering a set (rows) with subsets (columns)

Interlude 3: the feasibility test

Heuristic algorithms often require to solve the following problem

Given a subset x, is x feasible or not? In short, $x \in X$?

It is a decision problem

The feasibility test requires to compute from the solution and test

- a single number: the total volume (*KP*), the cardinality (*MDP*)
- a single set of numbers: values assigned to each variable (*Max-SAT*), number of machines for each task (*PMSP*)
- several sets of numbers: number of containers for each object and total volume of each container (*BPP*)

The time required can be different if the test is performed

- from scratch on a generic subset x
- on a subset x' obtained slightly modifying a feasible solution x

Some modifications can be forbidden *a priori* to avoid infeasibility (insertions and removals for *MDP*, *PMSP*, *Max-SAT*), while others require an *a posteriori* test (exchanges)

Numerical matrix problems: Set Packing

Given

- a binary matrix $A \in \mathbb{B}^{m,n}$ with row set R and column set C
- columns j' e $j'' \in C$ conflict with each other when $a_{ij'} = a_{ij''} = 1$
- a function $\phi : C \to \mathbb{N}$ provides the value of each column

Select a subset of nonconflicting columns of maximum value

The ground set is the set of columns: $B = C$

The feasible region includes all subsets of nonconflicting columns

$$X = \left\{ x \subseteq B : \sum_{j \in x} a_{ij} \leq 1 \; \forall i \in R \right\}$$

The objective is to maximize the total value of the selected columns

$$\max_{x \in X} f(x) = \sum_{j \in x} \phi_j$$

Example

ϕ	4	6	10	14	5	6

A						
	0	1	0	0	1	0
	0	0	1	1	0	0
	1	0	0	0	0	1
	0	0	0	1	1	1
	1	1	1	0	0	0

A							
	0	1	0	0	1	0	1
	0	0	1	1	0	0	1
	1	0	0	0	0	1	0
	0	0	0	1	1	1	1
	1	1	1	0	0	0	1

$$x' = \{c_2, c_4\} \in X$$

$$f(x') = 20$$

A							
	0	1	0	0	1	0	1
	0	0	1	1	0	0	0
	1	0	0	0	0	1	2
	0	0	0	1	1	1	2
	1	1	1	0	0	0	1

$$x'' = \{c_1, c_5, c_6\} \notin X$$

$$f(x'') = 15$$

"Set Packing": packing disjoint subsets (columns) of a set (rows)

Numerical matrix problems: Set Partitioning (*SPP*)

Given

- a binary matrix $A \in \mathbb{B}^{m,n}$ with a set of rows R and a set of columns C
- a function $c : C \to \mathbb{N}$ that provides the cost of each column

select a minimum cost subset of nonconflicting columns covering all rows

The ground set is the set of columns: $B = C$

The feasible region includes all subsets of columns that cover all rows and are not conflicting

$$X = \left\{ x \subseteq C : \sum_{j \in x} a_{ij} = 1 \; \forall i \in R \right\}$$

The objective is to minimize the total cost of the selected columns

$$\min_{x \in X} f(x) = \sum_{j \in x} c_j$$

Example

c	4	6	10	14	5	6

A						
	0	1	0	0	1	0
	0	0	1	1	0	0
	1	0	0	0	0	1
	0	0	0	1	1	0
	1	1	1	0	0	0

A							
	0	1	0	0	1	0	1
	0	0	1	1	0	0	1
	1	0	0	0	0	1	1
	0	0	0	1	1	0	1
	1	1	1	0	0	0	1

$$x' = \{c_2, c_4, c_6\} \in X$$

$$f(x') = 26$$

A							
	0	1	0	0	1	0	1
	0	0	1	1	0	0	0
	1	0	0	0	0	1	2
	0	0	0	1	1	0	1
	1	1	1	0	0	0	1

$$x'' = \{c_1, c_5, c_6\} \notin X$$

$$f(x'') = 15$$

"Set Partitioning": partition a set (rows) into subsets (columns)

Interlude 4: the search for feasible solutions

Heuristic algorithms often require to solve the following problem

Find a feasible solution $x \in X$

It is a search problem

Depending on the problem, the solution can be trivial:

- some sets are always feasible, such as $x = \emptyset$ (*KP*, *SPP*) or $x = B$ (feasible instances of *SCP*)
- random solutions satisfying a constraint, such as $|x| = k$ (*MDP*)
- random solutions satisfying consistency constraints, such as assigning one task to each machine (*PMSP*), one value to each logic variable (*Max-SAT*), etc. . .

but it can also be hard:

- in the *BPP* the number of containers must be sufficiently large (e. g., provide one container for each object, then minimize)
- in the *SPP* no polynomial algorithm is known to solve the problem

Some algorithms enlarge the feasible region from X to X' (relaxation)

- the objective f must be extended from X to X' (*see Interlude 1*)
- but often $X' \setminus X$ includes better solutions (*. . . how about that?*)

Graph problems: Vertex Cover (*VCP*)

Given an undirected graph $G = (V, E)$, select a subset of vertices of minimum cardinality such that each edge of the graph is incident to it

The ground set is the vertex set: $B = V$

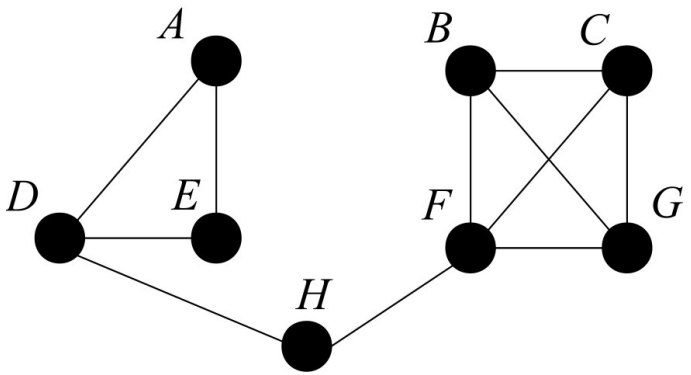
The feasible region includes all vertex subsets such that all the edges of the graph are incident to them

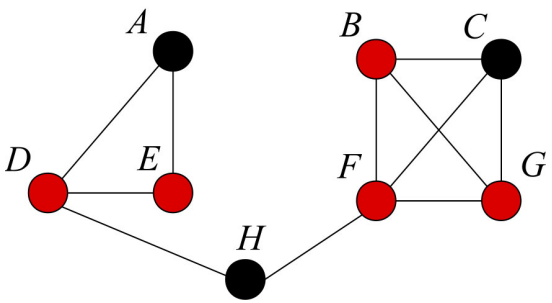
$$X = \left\{ x \subseteq V : x \cap (i,j) \neq \emptyset \; \forall \, (i,j) \in E \right\}$$

The objective is to minimize the number of selected vertices

$$\min_{x \in X} f(x) = |x|$$

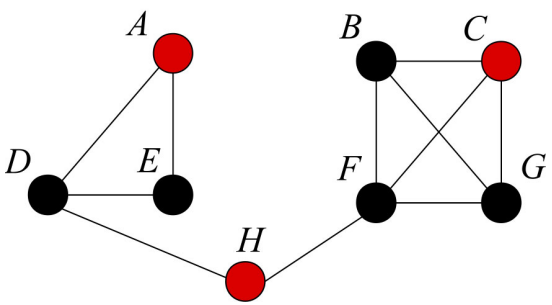
Example





$$x' = \{B, D, E, F, G\} \in X$$

$$f(x') = 5$$



$$x'' = \{A, C, H\} \notin X$$

$$f(x'') = 3$$

Graph problems: Maximum Clique Problem

Given

- an undirected graph $G = (V, E)$
- a function $w : V \to \mathbb{N}$ that provides the weight of each vertex

select the subset of pairwise adjacent vertices of maximum weight

The ground set is the vertex set: $B = V$

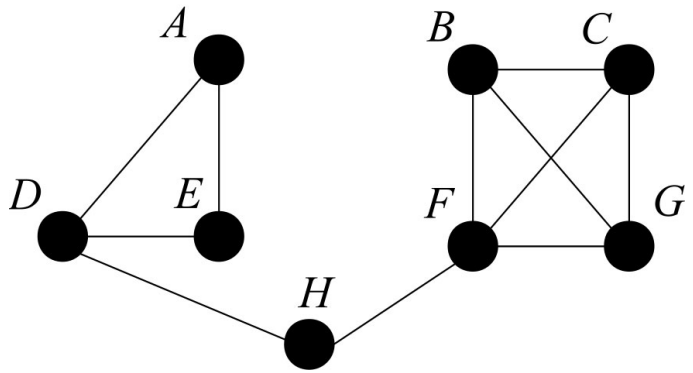
The feasible region includes all subsets of pairwise adjacent vertices

$$X = \left\{ x \subseteq V : (i, j) \in E \; \forall i \in x, \forall j \in x \setminus \{i\} \right\}$$

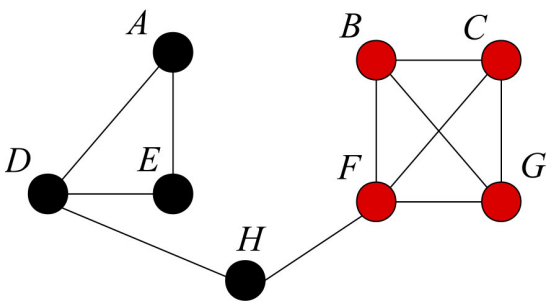
The objective is to maximize the weight of the selected vertices

$$\max_{x \in X} f(x) = \sum_{j \in x} w_j$$

Example

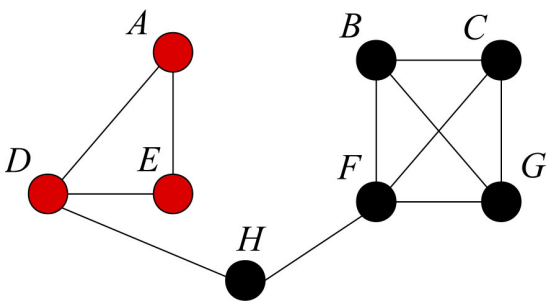


Uniform weights: $w_i = 1$ for each $i \in V$



$$x' = \{B, C, F, G\} \in X$$

$$f(x') = 4$$



$$x'' = \{A, D, E\} \in X$$

$$f(x'') = 3$$

Graph problems: Maximum Independent Set Problem

Given

- an undirected graph $G = (V, E)$
- a function $w : V \to \mathbb{N}$ that provides the weight of each vertex

select the subset of pairwise nonadjacent vertices of maximum weight

The ground set is the vertex set: $B = V$

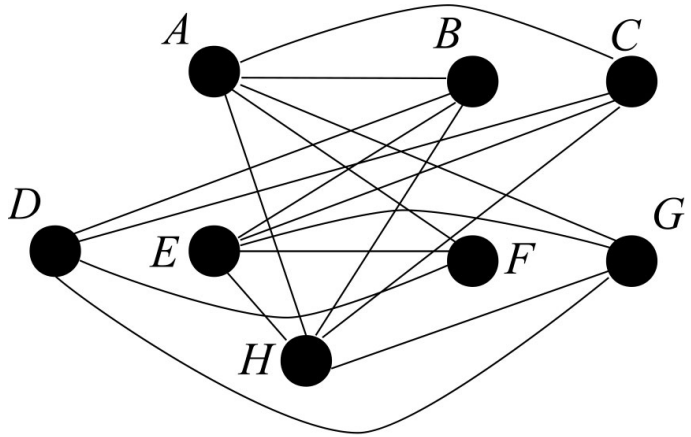
The feasible region includes the subsets of pairwise nonadjacent vertices

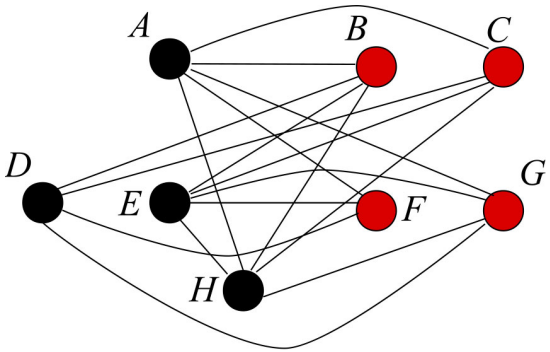
$$X = \left\{ x \subseteq B : (i, j) \notin E \; \forall i \in x, \forall j \in x \setminus \{i\} \right\}$$

The objective is to maximize the weight of the selected vertices

$$\max_{x \in X} f(x) = \sum_{j \in x} w_j$$

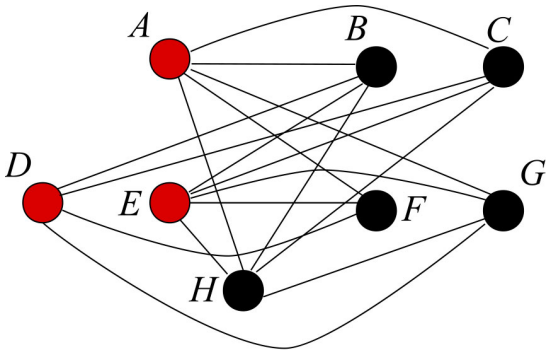
Example





$$x' = \{B, C, F, G\} \in X$$

$$f(x') = 4$$



$$x'' = \{A, D, E\} \in X$$

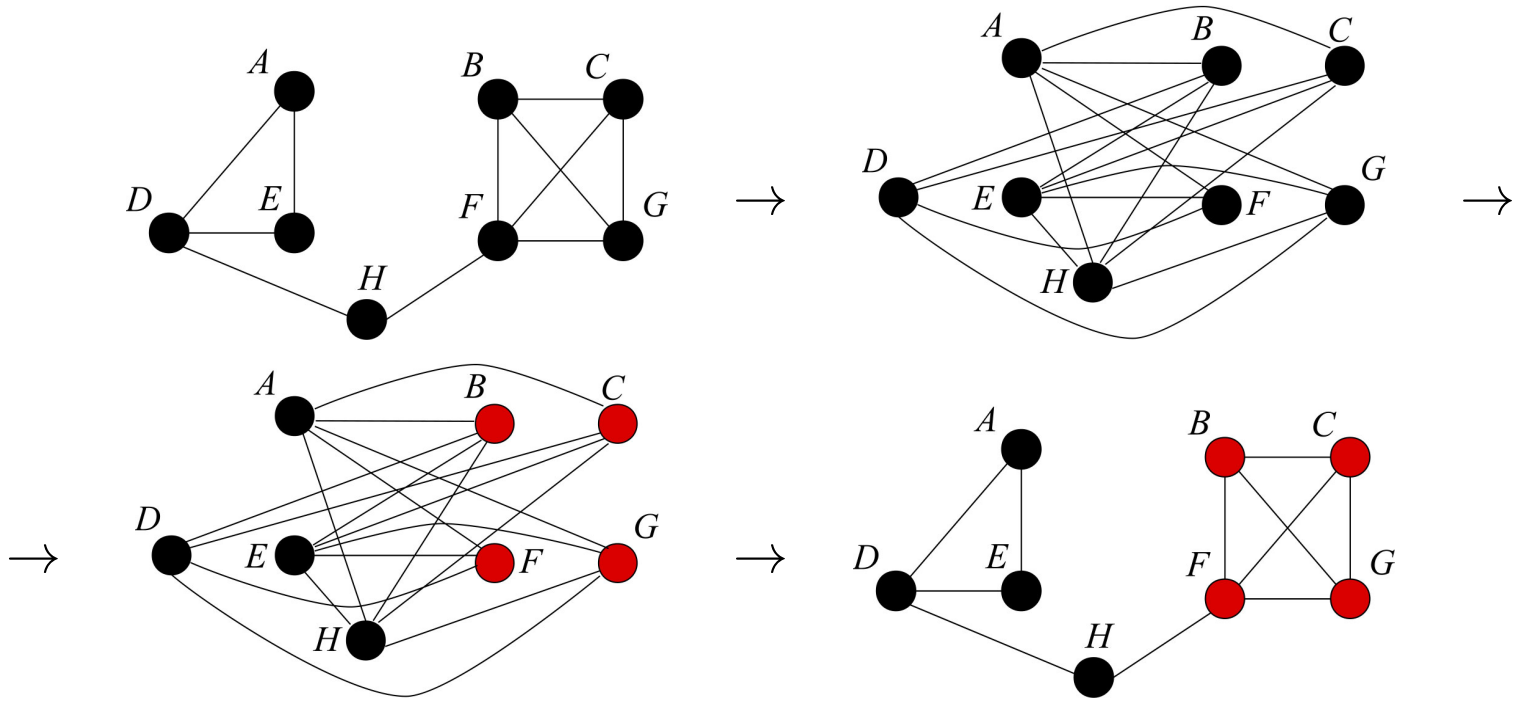
$$f(x'') = 3$$

Interlude 5: the relations between problems (1)

Each instance of the *MCP* is equivalent to an instance of the *MISP*

1. start from the *MCP* instance, that is graph $G = (V, E)$
2. build the complementary graph $\bar{G} = (V, (V \times V) \setminus E)$
3. find an optimal solution of the *MISP* on $\bar{G}$
4. the corresponding vertices give an optimal solution of the *MCP* on G

   (*a heuristic MISP solution gives a heuristic MCP solution*)

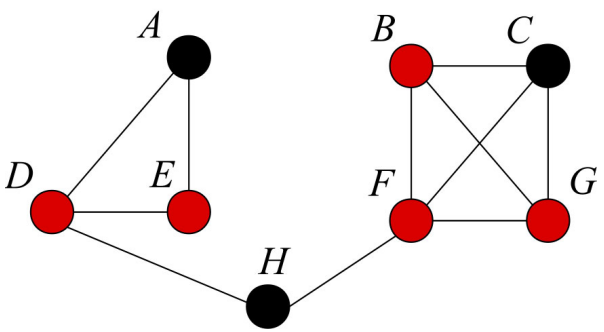


The process can be applied also in the opposite direction

Interlude 5: the relations between problems (2)

The *VCP* and the *SCP* are also related, but in a different way; each instance of the *VCP* can be transformed into an instance of the *SCP*:

- each edge i corresponds to a row of the covering matrix A
- each vertex j corresponds to a column of A
- if edge i touches vertex j, set $a_{ij} = 1$; otherwise $a_{ij} = 0$
- an optimal solution of the *SCP* gives an optimal solution of the *VCP*
  (*a heuristic SCP solution gives a heuristic VCP solution*)



	A	B	C	D	E	F	G	H
(A, D)	1	0	0	1	0	0	0	0
(A, E)	1	0	0	0	1	0	0	0
(B, C)	0	1	1	0	0	0	0	0
(B, F)	0	1	0	0	0	1	0	0
(B, G)	0	1	0	0	0	0	1	0
(C, F)	0	0	1	0	0	1	0	0
(C, G)	0	0	1	0	0	0	1	0
(D, E)	0	0	0	1	1	0	0	0
(D, H)	0	0	0	1	0	0	0	1
(F, G)	0	0	0	0	0	1	1	0
(F, H)	0	0	0	0	0	1	0	1

It is not simple to do the reverse

Interlude 5: the relations between problems (3)

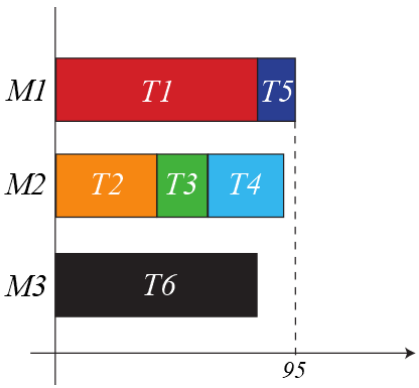
The *BPP* and the *PMSP* are equivalent, but in a more sophisticated way:

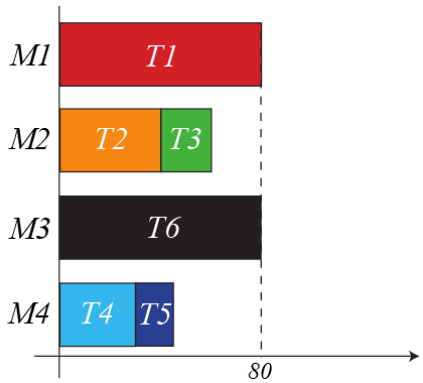
- the tasks correspond to the objects
- the machines correspond to the containers, but
  - *BPP*: minimize the number of containers, given the capacity
  - *PMSP*: given the number of machines, minimize the completion time

Start from a *BPP* instance

1. make an assumption on the optimal number of containers (e.g., 3)
2. build the corresponding *PMSP* instance
3. compute the optimal completion time (e.g., 95)
   - if it exceeds the capacity (e.g., 80), increase the assumption (4 or 5)
   - if it does not, decrease the assumption (2 or 1)

(*using heuristic PMSP solutions leads to a heuristic BPP solution*)





The reverse process is possible

The two problems are equivalent, but each one must be solved several times

Kernelization ("problem reduction")

Kernelization transforms all instances of P into simpler instances of P, instead of instances of another problem Q

This is also known as problem reduction

Quite often, in fact, useful properties allow to prove that

- there exists an optimal solution not including certain elements of B
  ($\Rightarrow$ *such elements can be removed*)
- there exists an optimal solution including certain elements of B
  ($\Rightarrow$ *such elements can be set apart and added later*)

In short, remove elements of B without affecting the solution

Possible useful outcomes are

- an exact algorithm polynomial in n (parameterized complexity)
- faster exact and heuristic algorithms
- better heuristic solutions
- heuristic kernelization: apply relaxed conditions sacrificing optimality

Kernelization of the *VCP*

Useful property: each vertex v of degree $\delta_v \geq k+1$ must belong to any feasible solution of value $\leq k$

Otherwise, $k+1$ edges should be covered each by a different vertex

Kernelization algorithm:

- start at step $t = 0$ with $k_0 = k$ and an empty vertex subset $x_t := \emptyset$
- set $t = t + 1$ and add to the solution the vertices of degree $\geq k_t + 1$

$$\delta_v \geq k_t + 1 \;\Rightarrow\; x_t := x_{t-1} \cup \{v\}$$

- update k_t: $k_t := k_0 - |x|$
- remove the vertices of zero degree, those of x and the covered edges

$$V := \{v \in V : \delta_v > 0\} \setminus x_t \qquad E := \{e \in E : e \cap x_t = \emptyset\}$$

- if $|E| > k_t^2$, there is no feasible solution (k_t *vertices are not enough*)
- if $|E| \leq k_t^2 \Rightarrow |V| \leq 2k_t^2$; apply the exhaustive algorithm

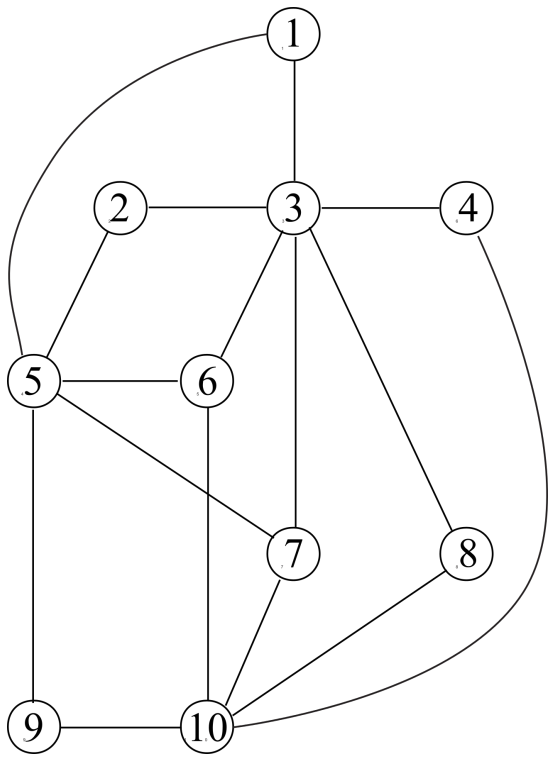
The complexity is $T(n,k) \in \Theta\left(n + m + 2^{2k^2} k^2\right)$

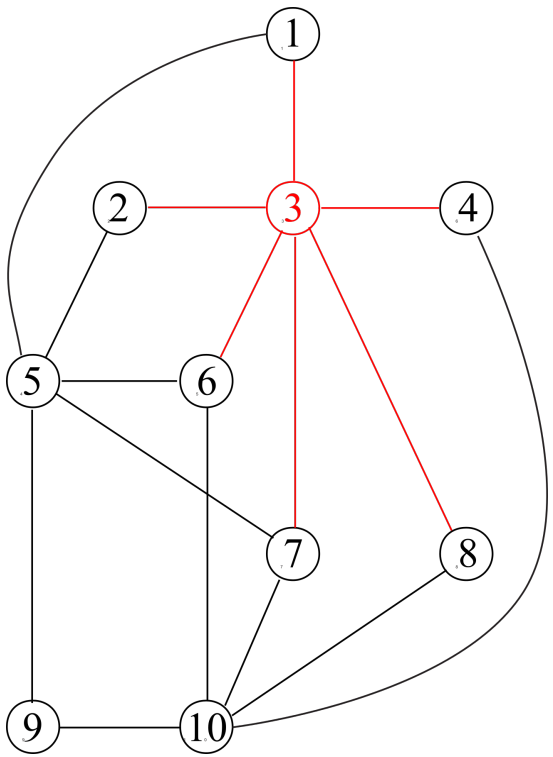
Kernelization of the *VCP*

Given the following graph, is there a solution with $k \leq k_0 = 5$?

Exhaustive algorithm: $T(n) \in \Theta(2^n(m+n))$
Since $n = 10$ and $m = 16$, $T(n) \approx 2^{10}(10+16) = 26\,624$

$\delta_3 = 6 \geq k_0 + 1 \Rightarrow x_1 := \{3\}$, remove the incident edges and $k_1 = 4$



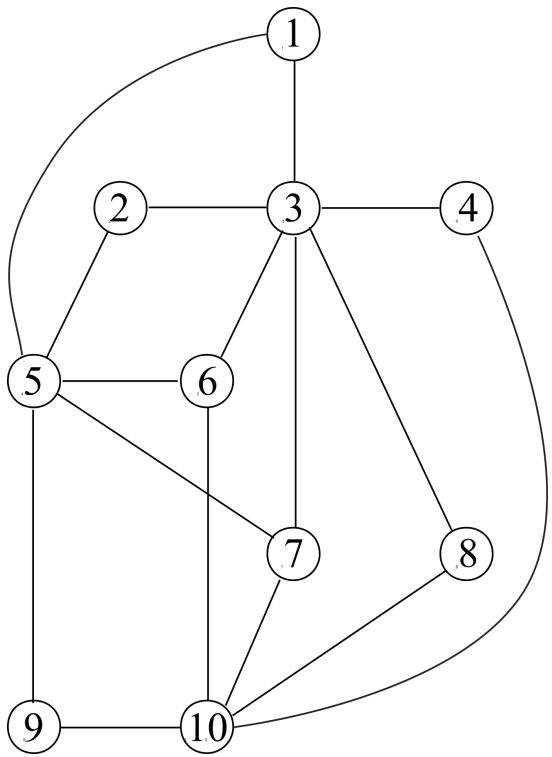


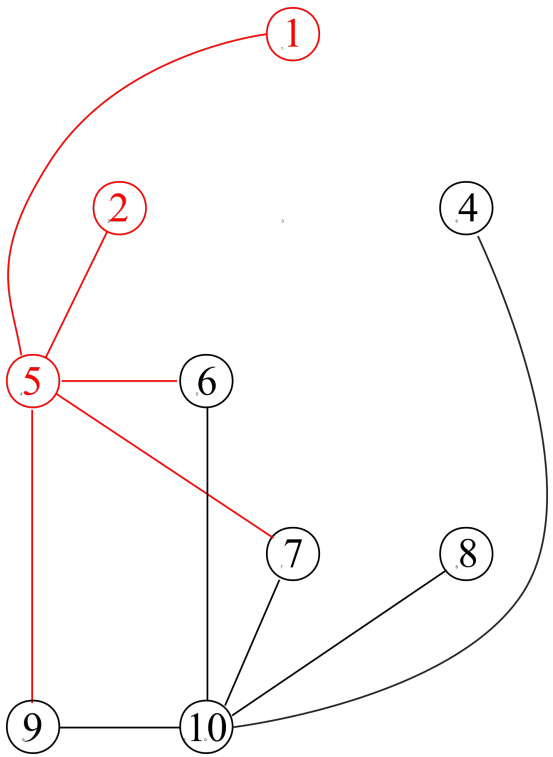
Kernelization of the *VCP*

Given the following graph, is there a solution with $k \leq k_0 = 5$?

Exhaustive algorithm: $T(n) \in \Theta(2^n(m+n))$
Since $n = 10$ and $m = 16$, $T(n) \approx 2^{10}(10+16) = 26\,624$

$\delta_5 = 5 \geq k_1 + 1 \Rightarrow x_2 := \{3, 5\}$, remove the incident edges and $k_2 = 3$



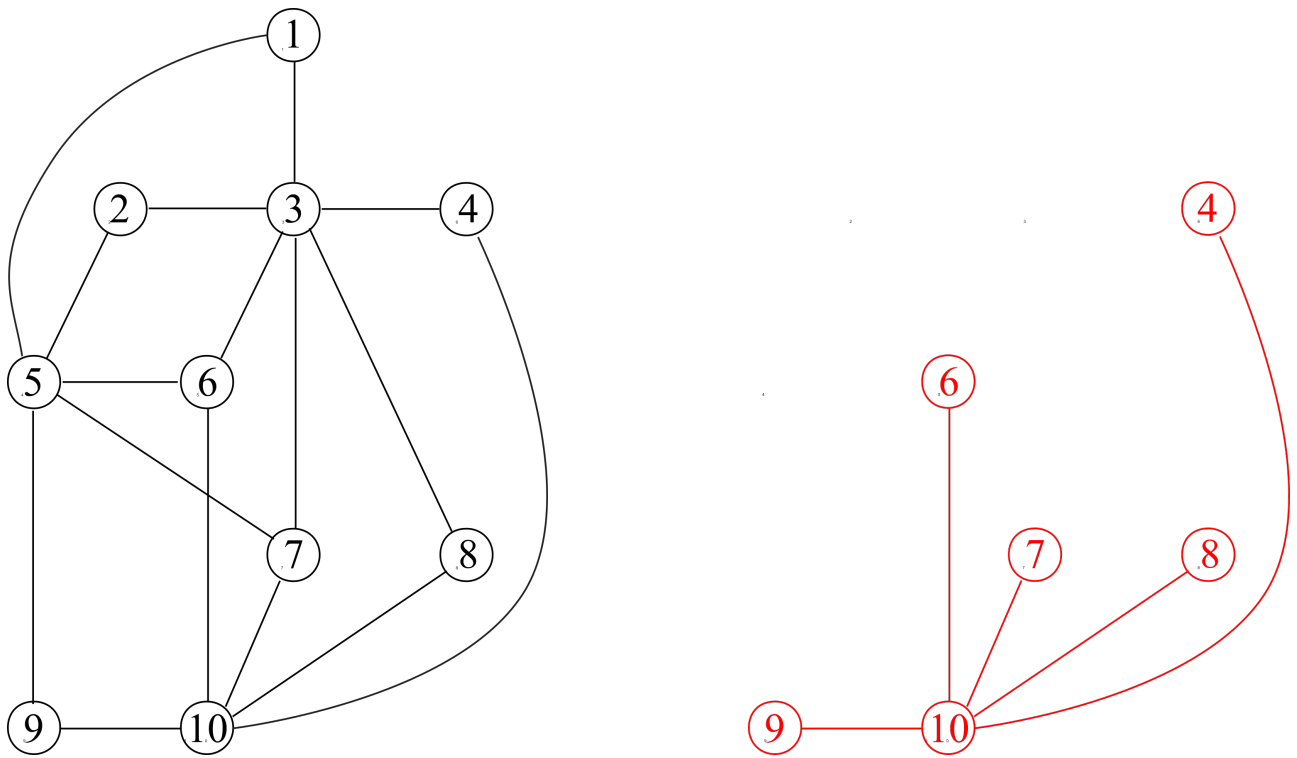


Kernelization of the *VCP*

Given the following graph, is there a solution with $k \leq k_0 = 5$?

Exhaustive algorithm: $T \in \Theta\left(2^n\left(m+n\right)\right)$
Since $n = 10$ and $m = 16$, $T \approx 2^{10}\left(10+16\right) = 26\,624$

$\delta_{10} = 5 \geq k_2 + 1 \Rightarrow x_3 := \{3, 5, 10\}$, remove the incident edges and $k_3 = 2$



Kernelization: $T \approx m + n = 10 + 16 = 26$

Graph problems: Travelling Salesman Problem (*TSP*)

Given

- a directed graph $G = (N, A)$
- a function $c : A \to \mathbb{N}$ that provides the cost of each arc

select a circuit visiting all the nodes of the graph at minimum cost

The ground set is the arc set: $B = A$

The feasible region includes the circuits that visit all nodes in the graph (hamiltonian circuits)

How to determine whether a subset is a feasible solution?

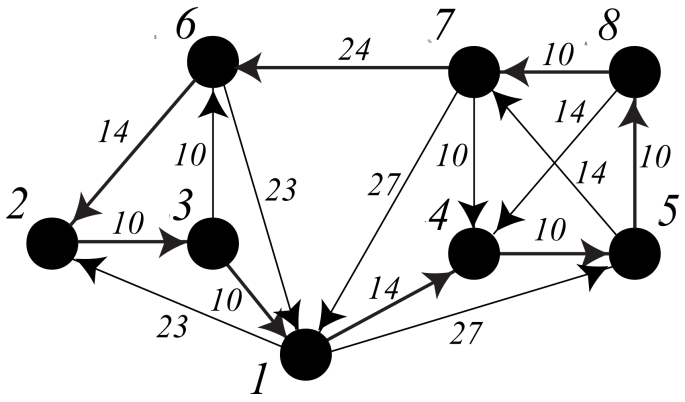
And a modification of a feasible solution?

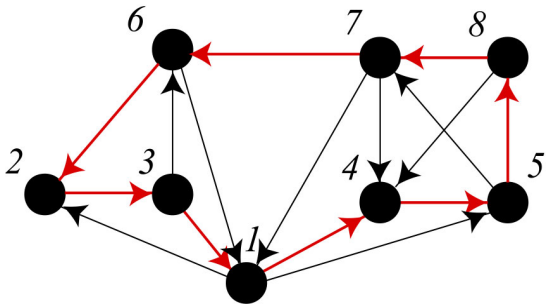
Is it hard to find a feasible solution?
(hard in general, trivial on a complete graph)

The objective is to minimize the total cost of the selected arcs

$$\min_{x \in X} f(x) = \sum_{j \in x} c_j$$

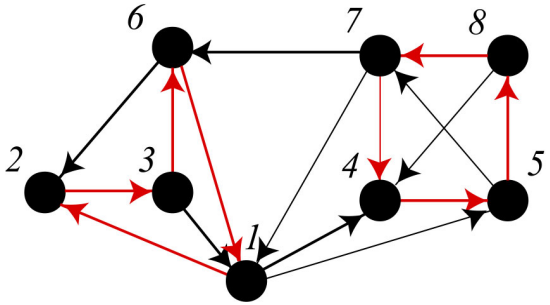
Example





$$x' = \{(1,4),(4,5),(5,8),(8,7),(7,6),(6,2),(2,3),(3,1)\} \in X$$

$$f(x') = 102$$



$$x'' = \{(4,5),(5,8),(8,7),(7,4),(1,2),(2,3),(3,6),(6,1)\} \notin X$$

$$f(x'') = 106$$

Graph problems: Capacitated Min. Spanning Tree Problem

Given

- an undirected graph $G = (V, E)$ with a root vertex $r \in V$
- a function $c : E \to \mathbb{N}$ that provides the cost of each edge
- a function $w : V \to \mathbb{N}$ that provides the weight of each vertex
- a number $W \in \mathbb{N}$ that is the capacity of each subtree

select a minimum cost spanning tree such that each branch (subtree appended to the root) respect the capacity

The ground set is the edge set: $B = E$

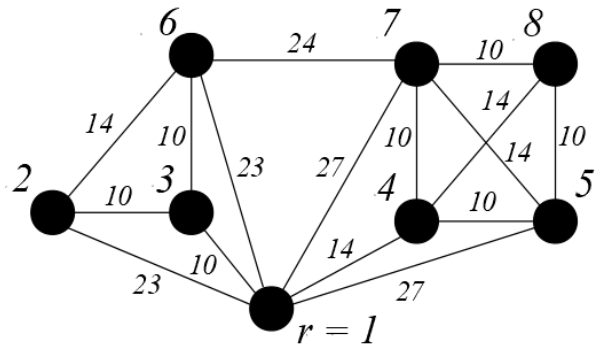
The feasible region includes all spanning trees such that the weight of the vertices spanned by each subtree appended to the root do not exceed W

The feasibility test requires to visit the subgraph

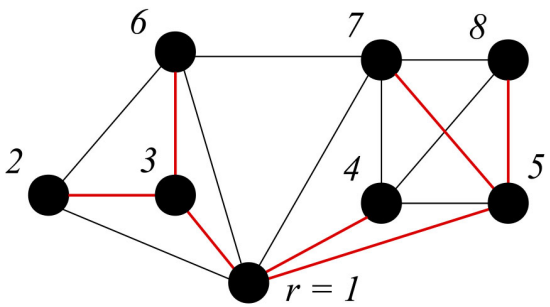
The objective is to minimize the total cost of the selected edges

$$\min_{x \in X} f(x) = \sum_{j \in x} c_j$$

Example

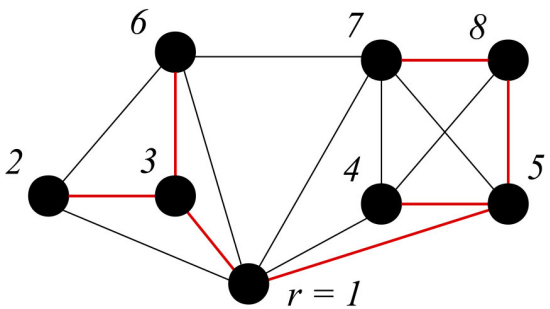


Uniform weight ($w_i = 1$ for each $i \in V$) and capacity: $W = 3$



$$x' = \{(r,3),(3,2),(3,6),(r,4),(r,5),(5,7),(5,8)\} \in X$$

$$f(x') = 95$$



$$x'' = \{(r,3),(3,2),(3,6),(r,5),(5,4),(5,8),(8,7)\} \notin X$$

$$f(x'') = 87$$

It is easy to evaluate the objective, less easy the feasibility

Cost of the main operations

The objective function is

- fast to evaluate: sum the edge costs
- fast to update: sum the added costs and subtract the removed ones

but it is easy to obtain subtrees that span vertices in a nonoptimal way

The feasibility test is

- not very fast to perform:
  - visit to check for connection and acyclicity
  - visit to compute the total weight of each subtree
- not very fast to update:
  - show that the removed edges break the loops introduced by the added ones
  - recompute the weights of the subtrees

This also holds when the graph is complete

What if we described the problem in terms of vertex subsets?

An alternative description

Define a set of subtrees T (*as the containers in the BPP*)

One for each vertex in $V \setminus \{r\}$*: some can be empty*

The ground set is the set of the (vertex,subtree) pairs: $B = V \times T$

The feasible region includes all partitions of the vertices into connected subsets (*visit; trivial on complete graphs*) of weight $\leq W$ (*as in the BPP*)

$$X = \left\{ x \subseteq B : |x \cap B_v| = 1 \; \forall v \in V \setminus \{r\}, \sum_{(i,j) \in B^t} w_i \leq W \; \forall t \in T, \ldots \right\}$$

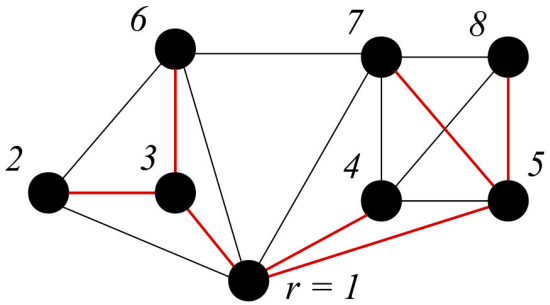
with $B_v = \{(i,j) \in B : i = v\}$, $B^t = \{(i,j) \in B : j = t\}$

The objective is to minimize the sum of the costs of the subtrees spanning each subset of vertices plus the edges connecting them to the root

It is a combination of minimum spanning tree problems

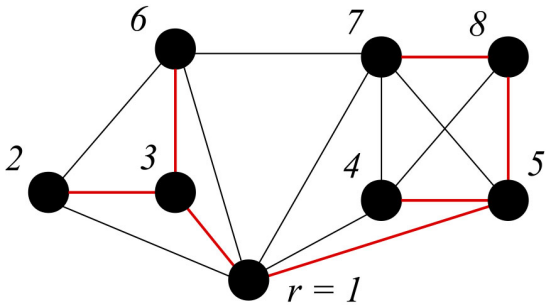
Example

The previously considered solutions now have a different representation



$$x' = \{(2,1),(3,1),(6,1),(4,2),(5,3),(7,3),(8,3)\} \in X$$

$$f(x') = 95$$



$$x'' = \{(2,1),(3,1),(6,1),(4,2),(5,2),(7,2),(8,2)\} \notin X$$

$$f(x'') = 87$$

The feasibility test only requires to sum the weights, computing the objective requires to solve a MST problem

Cost of the main operations

The objective function is

- slow to evaluate: compute a MST for each subset
- slow to update: recompute the MST for each modified subset

but the subtrees are optimal by construction

If the graph is complete, the feasibility test is

- fast to perform:
  - sum the weights of the vertices for each subtree
- fast to update:
  - sum the added weights and subtract the removed ones

Advantages and disadvantages switched places

Graph problems: Vehicle Routing Problem (*VRP*)

Given

- a directed graph $G = (N, A)$ with a depot node $d \in N$
- a function $c : A \to \mathbb{N}$ that provides the cost of each arc
- a function $w : N \to \mathbb{N}$ that provides the weight of each node
- a number $W \in \mathbb{N}$ that is the capacity of each circuit

select the set of minimum cost circuits that visit the depot and such that each one respects the capacity

The ground set could be

- the arc set: $B = A$
- the set of all (node,circuit) pairs: $B = N \times C$

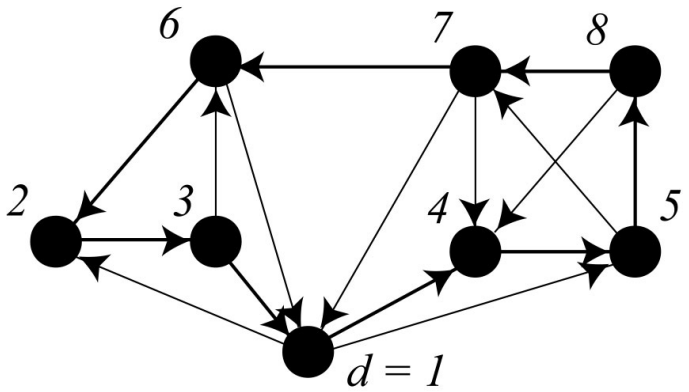
The feasible region could include

- all arc subsets that cover all nodes with circuits visiting the depot and whose weight does not exceed W (*again the visit of a graph*)
- all partitions of the nodes into subsets of weight non larger than W and admitting a spanning circuit ($\mathcal{NP}$-*hard problem!*)

The objective is to minimize the total cost of the selected arcs

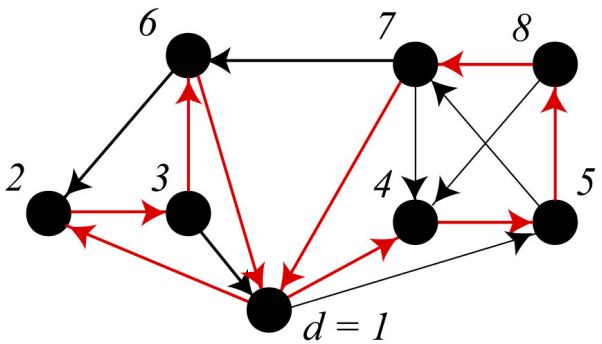
$$\min_{x \in X} f(x) = \sum_{j \in x} c_j$$

Example



Uniform weight ($w_i = 1$ for each $i \in N$) and capacity: $W = 4$

The solutions could be described as



- arc subsets
  $x = \{(d,2),(2,3),(3,6),(6,d),(d,4),$
  $(4,5),(5,8),(8,7),(7,d)\} \in X$
- node partitions
  $x = \{(2,1),(3,1),(6,1),$
  $(4,2),(5,2),(7,2),(8,2)\} \in X$

$f(x) = 137$

Interlude 6: combining alternative representations

The *CMSTP* and the *VRP* share an interesting complication:
different definitions of the ground set B are possible and natural

- the description as a set of edges/arcs
  looks preferable to manage the objective
- the description as a set of pairs (vertex,tree)/(node/circuit) looks better to generate optimal solutions and to deal with feasibility

Which description should be adopted?

- the one that makes easier the most frequent operations
- both, if they are used much more frequently than updated, so that the burden of keeping them up-to-date and consistent is acceptable