Heuristic Algorithms

Master's Degree in Computer Science/Mathematics

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Problems

Informally, a problem is a question on a system of mathematical objects

The same question can often be asked on many similar systems

- an instance $I \in \mathcal{I}$ is each specific system concerned by the question
- a solution $S \in \mathcal{S}$ is an answer corresponding to one of the instances

Example: "*is n a prime number?*" is a problem with infinite instances and two solutions ($\mathcal{I} = \mathbb{N}^+ \setminus \{1\}$ and $\mathcal{S} = \{\ \texttt{yes},\ \texttt{no}\ \}$)
instance $I = 7$ corresponds to solution $S_I = \texttt{yes}$
instance $I' = 10$ corresponds to solution $S_{I'} = \texttt{no}$
...

Formally, a problem is the function which relates instances and solutions

$$P : \mathcal{I} \to \mathcal{S}$$

Defining a function does not mean to know how to compute it

Algorithms

An algorithm is a formal procedure, composed by elementary steps, in finite sequence, each determined by an input and by the results of the previous steps

An algorithm for a problem P is an algorithm which, given in input $I \in \mathcal{I}$, returns in output $S_I \in \mathcal{S}$

$$A : \mathcal{I} \to \mathcal{S}$$

An algorithm defines a function plus the way to compute it; it is

- exact if its associated function coincides with the problem
- heuristic otherwise

A heuristic algorithm is useful if it is

1. efficient: it "costs" much less than an exact algorithm
2. effective: it "frequently" provides a solution "close" to the right one

This lesson deals with efficiency

Cost of a heuristic algorithm

The "cost" of an (exact or heuristic) algorithm denotes

- not the monetary cost to buy or implement it
- but the computational cost of running it
  - time required to terminate the finite sequence of elementary steps
  - space occupied in memory by the results of the previous steps

The time is much more discussed because

- the space is a renewable resource, the time is not
- using space requires to use at least as much time
- it is technically easier to distribute the use of space than of time

Space and time are partly interchangeable:
it is possible to reduce the use of one by increasing the use of the other

A useful measure of time

The time required to solve a problem depends on several aspects

- the specific instance to solve
- the algorithm used
- the machine running the algorithm
- ...

Our measure of the computational time should be

- unrelated to technology, that is the same for different machines
- concise, that is summarized in a simple symbolic expression
- ordinal, that is sufficient to compare different algorithms

The computational time in seconds for each instance violates all requisites

Worst-case asymptotic time complexity

The worst-case asymptotic complexity of an algorithm (nearly) provides such a measure through the following passages

1. define time as the number T of elementary operations performed (that is a value independent from the specific computer)
2. define the size of an instance as a suitable value n (e.g., the number of elements of the ground set, variables or formulae of the CNF, rows or columns of the matrix, nodes or arcs of the graph)
3. find the worst-case, i. e. the maximum of T on all instances of size n

$$T(n) = \max_{I \in \mathcal{I}_n} T(I) \qquad n \in \mathbb{N}$$

(*now time complexity is only a function* $T : \mathbb{N} \to \mathbb{N}$)

4. approximate $T(n)$ from above and/or below with a simpler function $f(n)$, considering only their asymptotic behaviour (for $n \to +\infty$)
   (*the algorithm should be efficient on instances of large size*)
5. collect the functions in classes with the same approximating function
   (*the approximation relation is an equivalence relation*)

$$T(n) \in \Theta(f(n))$$

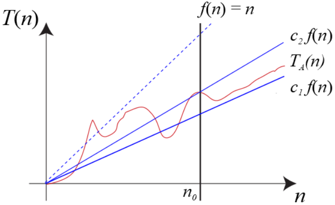
formally means that

$$\exists c_1, c_2 \in \mathbb{R}^+, n_0 \in \mathbb{N} : c_1 f(n) \leq T(n) \leq c_2 f(n) \text{ for all } n \geq n_0$$

where c_1, c_2 and n_0 are independent from n

$T(n)$ is *"enclosed"* between $c_1 f(n)$ and $c_2 f(n)$

- for some *"small"* value of c_1
- for some *"large"* value of c_2
- for some *"large"* value of n_0
- for some definition of *"small"* *and "large"*



Asymptotically, $f(n)$ estimates $T(n)$ up to a multiplying factor:

- for large instances, the computational time is at least and at most proportional to the values of function $f(n)$

The O functional spaces

$$T(n) \in O(f(n))$$

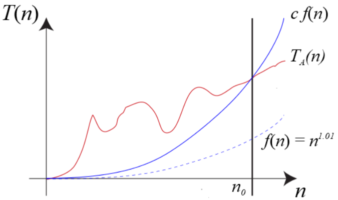
formally means that

$$\exists c \in \mathbb{R}^+, n_0 \in \mathbb{N} : T(n) \leq c\, f(n) \text{ for all } n \geq n_0$$

where c, and n_0 are independent from n

$T(n)$ is *"dominated"* by $c\, f(n)$

- for some *"large"* value of c
- for some *"large"* value of n_0
- for some definition of *"small"* *and* *"large"*



Asymptotically, $f(n)$ overestimates $T(n)$ up to a multiplying factor:

- for large instances, the computational time is at most proportional to the values of function $f(n)$

The Ω functional spaces

$$T(n) \in \Omega(f(n))$$

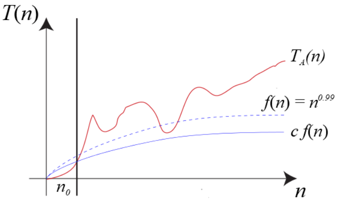
formally means that

$$\exists c > 0, n_0 \in \mathbb{N} : T(n) \geq c\, f(n) \text{ for all } n \geq n_0$$

where c and n_0 are independent from n

$T(n)$ *"dominates"* $c\, f(n)$

- for some *"small"* value of c
- for some *"large"* value of n_0
- for some definition of *"small" and "large"*



Asymptotically, $f(n)$ underestimates $T(n)$ up to a multiplying factor:

- for large instances, the computational time is at least proportional to the values of function $f(n)$

The exhaustive algorithm

For Combinatorial Optimization problems the size of an instance can be measured by the cardinality of the ground set

$$n = |B|$$

The exhaustive algorithm

- considers each subset $x \subseteq B$, that is each $x \in 2^{|B|}$
- tests its feasibility $(x \in X)$ in time $\alpha(n)$
- in the positive case, it evaluates the objective $f(x)$ in time $\beta(n)$
- if necessary, it updates the best value found so far

The time complexity of the exhaustive algorithm is

$$T(n) \in \Theta\left(2^n\left(\alpha(n) + \beta(n)\right)\right)$$

that is at least exponential, even if $\alpha(n)$ and $\beta(n)$ are small polynomials (which is the most frequent case)

Most of the time, the exhaustive algorithm is impractical

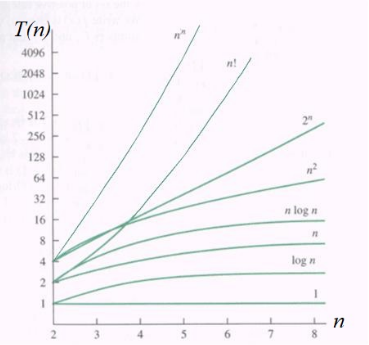
Polynomial and exponential complexity

In Combinatorial Optimization, the main distinction is between

- polynomial complexity: $T(n) \in O\left(n^d\right)$ for a constant $d > 0$
- exponential complexity: $T(n) \in \Omega\left(d^n\right)$ for a constant $d > 1$

The first family includes efficient algorithms, the second inefficient ones

In general, the heuristic algorithms are polynomial algorithms
for problems whose known exact algorithms are all exponential



Assuming 1 operation/μsec

n	n^2 op.	2^n op.
1	1μ sec	2μ sec
10	0.1 msec	1 msec
20	0.4 msec	1 sec
30	0.9 msec	17.9 min
40	1.6 msec	12.7 days
50	2.5 msec	35.7 years
60	3.6 msec	366 centuries

Problem transformations and reductions

A relation between problems allows to design algorithms (*Interlude 5*):

- by transformation:
  1. given I_P, (instance of P) build I_Q (instance of Q)
  2. given I_Q, apply algorithm A_Q to obtain S_Q (solution of I_Q)
  3. given S_Q, build S_P (solution of I_P)
- by reduction: repeat the transformation 1-2-3 several times correcting I_Q based on the solutions $\{S_Q\}$ already obtained

If A_Q is exact/heuristic, the overall algorithm A_P is exact/heuristic

The two algorithms often have a similar complexity:
if A_Q is polynomial/exponential and

1. building I_Q takes polynomial time
2. the number of iterations is polynomial
3. building S_P takes polynomial time

then A_P is polynomial/exponential

Beyond the worst-case complexity

The worst-case complexity

- cancels all information on the easier instances
  (*how are they made? how many are they?*)
- gives a rough overestimate of the computational time,
  in some (rare) cases useless
  (*see the simplex algorithm for Linear Programming*)

What if the hard instances are rare in the practical applications?

To compensate, one can investigate

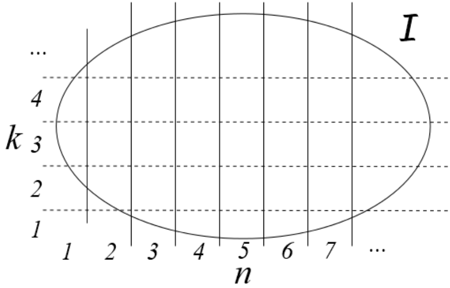
- the parameterized complexity, that is introduce some other relevant parameter k (besides the size n) and express the time as $T(n,k)$
- the average-case complexity, that is assume a probability distribution on $\mathcal{I}$ and express the time as the expected value

$$T(n) = E\left[T(I) \,|\, I \in \mathcal{I}_n\right]$$

Parameterized complexity

Some algorithms are exponential in k and polynomial in n, and therefore

- efficient on instances with low k
- inefficient on instances with large k



Nature of the additional parameter

If the additional parameter k is a part of the input, such as

- a numerical constant (e. g., the capacity in the *KP*)
- the maximum number of literals per formula in logic function problems
- the number of nonzero elements in numerical matrix problems
- the maximum degree, the diameter, etc... in graph problems

one knows *a priori* whether the algorithm is efficient on a given instance

If the additional parameter k is a part of the solution, such as

- its cardinality (as in the *VCP*)

one will only find out *a posteriori*

(*but an a priori estimate could be available*)

An example: the *VCP*

Exhaustive algorithm: for each of the 2^n subsets of vertices, test if it covers all edges, compute its cardinality and keep the smallest one

$$T(n, m) \in \Theta\left(2^n (m + n)\right)$$

(m *can be removed observing that* $m \leq n(n-1)/2$)

But if we already know a solution with $f(x) = |x| = k + 1$,
we can look for a solution of k vertices, and progressively decrease k

(*even better, use binary search on* k)

Naive algorithm: for each subset of k vertices, test if it covers all edges

$$T(n, m, k) \in \Theta\left(n^k m\right)$$

For fixed k, this algorithm is polynomial (*but in general very slow*)

Bounded tree search for the *VCP*

A better algorithm can be based on the following useful property

$$x \cap (u, v) \neq \emptyset \text{ for all } x \in X, (u, v) \in E$$

Any feasible solution includes at least one extreme vertex for each edge

Bounded tree search algorithm to find x with $|x| \leq k$:

1. choose any (u, v): either $u \in x$ or $u \notin x$ and $v \in x$
2. for each open case, remove the vertices of x and edges they cover

$$V := V \setminus x \qquad E := E \setminus \{e \in E : e \cap x \neq \emptyset\}$$

(*The edges covered by vertices in x are no longer constraining*)

3. if $|x| \leq k$ and $E = \emptyset$, x is the required solution
4. if $|x| = k$ and $E \neq \emptyset$, there is no solution
5. otherwise go to step 1

The complexity is $T(n, m, k) \in \Theta\left(2^k m\right)$, polynomial in n $(m < n^2)$

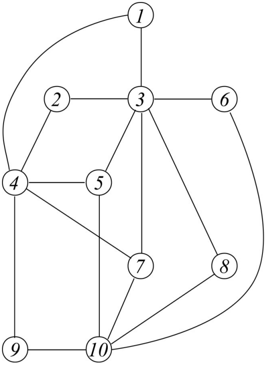
For $n \gg 2$, this algorithm is much more efficient than the naive one

Example

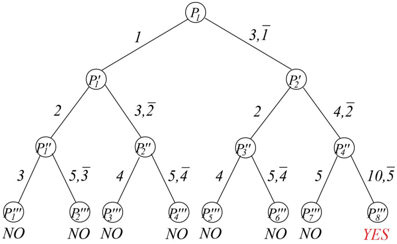
In the following graph $n = 10$, $m = 16$: is there a solution with $|x| \leq 3$?

Exhaustive algorithm: $\Theta\left(2^n (m+n)\right)$, with $2^n (m+n) = 1024 \cdot (16+10)$

Naive algorithm: $\Theta\left(n^k m\right)$, with $n^k m = 1\,000 \cdot 16$



Bounded tree search algorithm: $\Theta\left(2^k m\right)$
with $2^k m = 8 \cdot 16$



(*edges selected in lexicographic order*)

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

If $\delta_v \geq k+1$, vertex v belongs to any feasible solution of value $\leq k$

(*v has $k+1$ incident edges that should be covered by as many vertices*)

Kernelization algorithm to keep only vertices of solutions x with $|x| \leq k$:

- 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: $k_t := k_0 - |x_t|$
- 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 $T(n,k) \in \Theta\left(n + m + 2^{2k^2} k^2\right)$

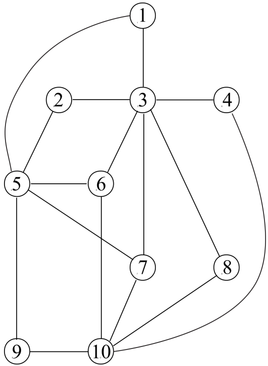
Example

Given the following graph, is there a solution with $|x| \leq k_0 = 5$?
$(n = 10,\ m = 16)$

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

Naive algorithm: $\Theta\left(n^k m\right) \Rightarrow T \approx 10^5 \cdot 16 = 16\,000\,000$

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



Example

Given the following graph, is there a solution with $|x| \leq k_0 = 5$?
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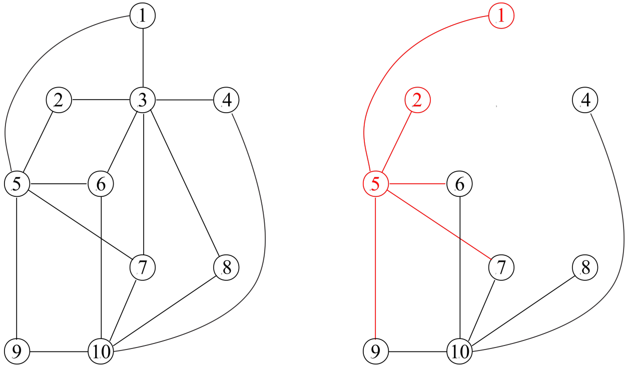
Exhaustive algorithm: $\Theta\left(2^n\,(m+n)\right) \Rightarrow T \approx 2^{10}\,(10+16) = 26\,624$

Naive algorithm: $\Theta\left(n^k m\right) \Rightarrow T \approx 10^5 \cdot 16 = 16\,000\,000$

$\delta_5 = 5 \geq k_1 + 1 \Rightarrow x_1 := \{3, 5\}$, remove the incident edges and $k_2 = 3$



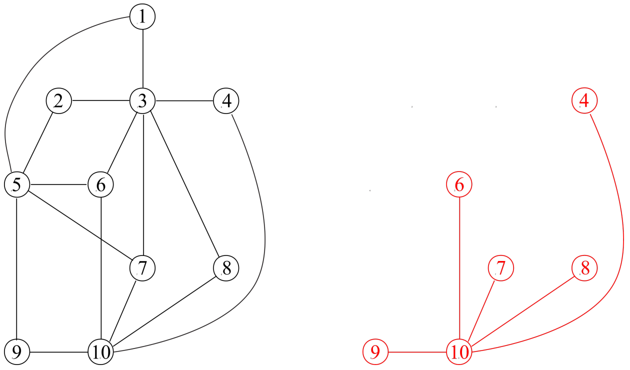
Example

Given the following graph, is there a solution with $|x| \leq k_0 = 5$?
$(n = 10,\ m = 16)$

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

Naive algorithm: $\Theta\left(n^k m\right) \Rightarrow T \approx 10^5 \cdot 16 = 16\,000\,000$

$\delta_{10} = 5 \geq k_2 + 1 \Rightarrow x_1 := \{3, 5, 10\}$, remove the incident edges and $k_3 = 2$



Kernelization: $\Theta\left(n+m\right) \Rightarrow T \approx 10+16 = 26$

Average-case complexity

Some algorithms are inefficient only on very few instances
(*see the simplex algorithm for Linear Programming*)

Theoretical studies

- define a probabilistic model of the problem,
  that is a probability distribution on $\mathcal{I}_n$ for each $n \in \mathbb{N}$
  typically quite simple (e.g., equiprobability, that is full ignorance)
- compute the expected value of $T(I)$

$$T(n) = E[T(I) | I \in \mathcal{I}_n]$$

Empirical studies

- build a simulation model of the problem,
  that is a probability distribution on $\mathcal{I}_n$ for each $n \in \mathbb{N}$
  theoretical or empirical (drawn from real-world data)
- build a benchmark of random instances according to the distribution
- apply the algorithm and measure the time required

Probabilistic models for numerical matrices

Binary random matrix with a given size (m rows and n columns)

1. equiprobability: list all 2^{mn} binary matrices and select one of the matrices with uniform probability
2. uniform probability: set each cell to 1 with a given probability p

$$Pr\left[a_{ij} = 1\right] = p \qquad (i = 1, \ldots, m;\ j = 1, \ldots, n)$$

If $p = 0.5$, it coincides with the equiprobability model, for other values some instances are more likely than others

3. fixed density: extract δmn cells out of mn with uniform probability and set them to 1

If $\delta = p$, it resembles the uniform probability model, but some instances cannot be generated

Probabilistic models for graphs

Random graph with a given number of vertices n

1. equiprobability: list all $2^{\frac{n(n-1)}{2}}$ graphs and
select one of the graphs with uniform probability
2. Gilbert's model, or uniform probability $G(n,p)$:

$$Pr[(i,j) \in E] = p \qquad (i \in V, j \in V \setminus \{i\})$$

All graphs with the same number of edges m have the same probability $p^m (1-p)^{\frac{n(n-1)}{2}-m}$ (different for each m)

If $p = 0.5$, it coincides with the equiprobability model
3. Erdős-Rényi model $G(n,m)$: extract m unordered vertex pairs out of $\frac{n(n-1)}{2}$ with uniform probability and create an edge for each one

If $\frac{2\,m}{n(n-1)} = p$, it resembles the uniform probability model,
but some instances cannot be generated

Probabilistic models for logic functions

Random CNF with a given number of variables n
and a given number of literals k for each logic formula

1. fixed-probability ensemble:
   list all $\binom{n}{k}2^k$ formulae of k distinct and consistent literals and add each one to the CNF with probability p
2. fixed-size ensemble:
   build m formulae, adding to each one k distinct and consistent literals, extracted with uniform probability

   If $p = \dfrac{m}{\binom{n}{k}2^k}$, *it resembles the fixed-probability model, but some instances cannot be generated*

Phase transitions

Different values of the (deterministic or probabilistic) parameters correspond to different regions of the instance set

For graphs

- $m = 0$ and $p = 0$ correspond to empty graphs
- $m = \frac{n(n-1)}{2}$ and $p = 1$ correspond to complete graphs
- intermediate values correspond to graphs of intermediate density (deterministically for m, probabilistically for p)

For many problems the performance of algorithms is strongly different in different regions concerning

- the computational time (for exact and heuristic algorithms)
- the quality of the solution (for heuristic algorithms)

Often, the performance variation takes place abruptly in small regions of the parameter space, as in phase transitions of physical systems

This is useful to predict the behaviour of an algorithm on a given instance

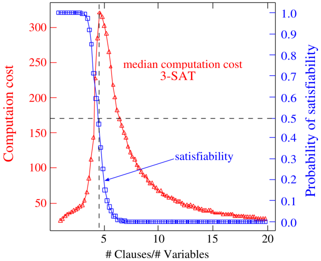
Phase transitions for 3-*SAT* and *Max*-3-*SAT*

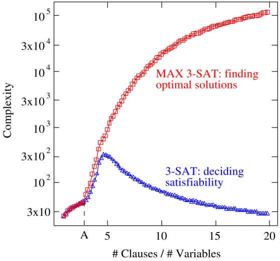
Given a *CNF* on n variables, with logic formulae containing 3 literals

- 3-*SAT*: is there a truth assignment satisfying all formulae?
- *Max*-3-*SAT*: what is the maximum number of satisfiable formulae?

As the formulae/variables ratio, $\alpha = m/n$ increases

- satisfiable instances decrease from nearly all (many variables for few formulae) to nearly none (few variables for many formulae)
- the computing time first sharply increases, then decreases for *SAT*, increases further for *Max-SAT* (*using a well-known exact algorithm*)





As $n \to +\infty$, the transition concentrates around $\alpha_c \approx 4.26$

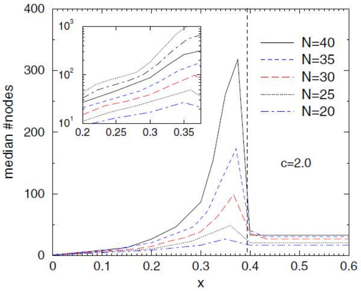
Phase transitions for the *VCP*

The *VCP* exhibits a similar phase transition as $\frac{|x|}{|V|}$ increases

- the computational time first explodes, then drops

  (*using a well-known exact algorithm*)

- as $n \to +\infty$ the transition concentrates around a critical value



When $|x|/|V|$ is small, some vertices are clearly necessary: problem solved when $|x|/|V|$ is large, many vertices are clearly necessary: problem solved

Computational cost of heuristic algorithms

The time complexity of a heuristic algorithm is usually

- strictly polynomial (with low exponents)
- fairly robust with respect to secondary parameters

Therefore, the worst-case estimation is also good on average

Metaheuristics use random steps or memory

- the complexity is well defined for single components of the algorithm
- the overall complexity is not clearly defined
  - in theory, it could extend indefinitely (but the pseudorandom number generator or the memory configurations would yield an infinite loop)
  - in practice, it is defined by a condition imposed by the user

(*more about this later*)

Conclusions

Why discussing these topics in a course on heuristics?

1. to guide the search for the correct algorithm: an exact algorithm can be efficient in a specific case, though inefficient in the worst one
2. to show that exact and heuristic algorithms can interact proficuously: heuristic algorithms provide information to improve exact algorithms (*they become more efficient*)
3. to show that kernelization improves also heuristic algorithms (*they become more efficient and more effective*)
4. to identify *a priori* the harder instances (*of course, not all algorithms have the same hard instances*)