## Heuristic Algorithms

## Master's Degree in Computer Science/Mathematics

## Roberto Cordone

DI - Università degli Studi di Milano


Schedule: $\quad$ Thursday 14.30-16.30 in classroom 201
Friday 14.30-16.30 in classroom 100
Office hours: on appointment
E-mail: roberto.cordone@unimi.it
Web page: https://homes.di.unimi.it/cordone/courses/2023-ae/2023-ae.html
Ariel site: https://rcordoneha.ariel.ctu.unimi.it

Lesson 4: Theoretical performance evaluation
Milano, A.A. 2023/24

## Effectiveness of a heuristic algorithm

A heuristic algorithm is useful if it is
(1) efficient: it "costs" much less than an exact algorithm
(2) effective: it "frequently" returns a solution "close to" an exact one

Let us now discuss the effectiveness of heuristic algorithms:

- closeness of the solution obtained to an optimal one
- frequency of hitting optimal or nearly optimal solutions

These features can be combined into a

- frequency distribution of solutions more or less close to the optimum

The effectiveness of a heuristic algorithm can be investigated with a

- theoretical analysis (a priori), proving that the algorithm finds always or with a given frequency solutions with a given guarantee of quality
- experimental analysis (a posteriori), measuring the performance of the algorithm on sampled benchmark instances to show that a guarantee of quality is respected in practice


## Indices of effectiveness

The effectiveness of a heuristic optimisation algorithm $A$ is measured by the difference between the heuristic value $f_{A}(I)$ and the optimum $f^{*}(I)$

- absolute difference:

$$
\tilde{\delta}_{A}(I)=\left|f_{A}(I)-f^{*}(I)\right| \geq 0
$$

rarely used, and only when the objective is a pure number

- relative difference:

$$
\delta_{A}(I)=\frac{\left|f_{A}(I)-f^{*}(I)\right|}{f^{*}(I)} \geq 0
$$

frequent in experimental analysis (usually as a percent ratio)

- approximation ratio:

$$
\rho_{A}(I)=\max \left[\frac{f_{A}(I)}{f^{*}(I)}, \frac{f^{*}(I)}{f_{A}(I)}\right] \geq 1
$$

frequent in theoretical analysis: the first form is used for minimisation problems, the second one for maximisation problems

## Theoretical analysis (in the worst case)

To obtain a compact measure, independent from $I$, find the worst case (as for efficiency, that is complexity)
The difference between $f_{A}(I)$ and $f^{*}(I)$ is in general unlimited, but for some algorithms it is limited:

- absolute approximation:

$$
\exists \tilde{\alpha}_{A} \in \mathbb{N}: \tilde{\delta}_{A}(I) \leq \tilde{\alpha}_{A} \text { for each } I \in \mathcal{I}
$$

A (rare) example is Vizing's algorithm for Edge Coloring ( $\tilde{\alpha}_{A}=1$ )

- relative approximation:

$$
\exists \alpha_{A} \in \mathbb{R}^{+}: \rho_{A}(I) \leq \alpha_{A} \text { for each } I \in \mathcal{I}
$$

Factor $\alpha_{A}\left(\tilde{\alpha}_{A}\right)$ is the relative (absolute) approximation guarantee
For other algorithms, the guarantee depends on the instance size

$$
\rho_{A}(I) \leq \alpha_{A}(n) \text { for each } I \in \mathcal{I}_{n}, n \in \mathbb{N}
$$

Effectiveness can be independent from size (contrary to efficiency)

## How to achieve an approximation guarantee?

For a minimisation problem, the aim is to prove that

$$
\exists \alpha_{A} \in \mathbb{R}: f_{A}(I) \leq \alpha_{A} f^{*}(I) \text { for each } I \in \mathcal{I}
$$

(1) find a way to build an underestimate $L B(I)$

$$
L B(I) \leq f^{*}(I) \quad I \in \mathcal{I}
$$

(2) find a way to build an overestimate $U B(I)$, related to $L B(I)$ by a coefficient $\alpha_{A}$

$$
U B(I)=\alpha_{A} L B(I) \quad I \in \mathcal{I}
$$

(3) find an algorithm $A$ whose solution is not worse than $U B(I)$

$$
f_{A}(I) \leq U B(I) \quad I \in \mathcal{I}
$$

Then $f_{A}(I) \leq U B(I)=\alpha_{A} L B(I) \leq \alpha_{A} f^{*}(I)$, for each $I \in \mathcal{I}$

$$
f_{A}(I) \leq \alpha_{A} f^{*}(I) \text { for each } I \in \mathcal{I}
$$

## A 2-approximated algorithm for the VCP

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

A matching is a set of nonadjacent edges
Maximal matching is a matching such that any other edge of the graph is adjacent to one of its edges (it cannot be enlarged)

Matching algorithm:
(1) Build a maximal matching $M \subseteq E$ scanning the edges of $E$ and including in $M$ those not adjacent to $M$

$$
\text { (now every edge of } E \backslash M \text { is adjacent to an edge of } M \text { ) }
$$

(2) The set of extreme vertices of the matching edges is a VCP solution

$$
x_{A}:=\bigcup_{(u, v) \in M}\{u, v\}
$$

and it can be improved removing the redundant vertices

## Example



The optimum is $f^{*}=5$

The matching algorithm is 2-approximated
(1) The cardinality of matching $M$ is an underestimate $L B(I)$

- the cardinality of an optimal covering for any subset of edges $E^{\prime} \subseteq E$ does not exceed that of an optimal covering for $E$

$$
\left|x_{E^{\prime}}^{*}\right| \leq\left|x_{E}^{*}\right|
$$

(it costs more to cover all edges than only the matching)

- the optimal covering of a matching $M$ has cardinality $|M|$
(each edge of the matching requires exactly one different vertex)
(2) Including both the extremes of each edge of the matching yields
- an overestimate (it covers both the matching and the adjacent edges)
- of value $U B(I)=2 L B(I)$ (two different vertices for each edge)
(3) The matching algorithm returns solutions of value $f_{A}(I) \leq U B(I)$
(possibly removing redundant vertices)
This implies $f_{A}(I) \leq 2 f^{*}(I)$ for each $I \in \mathcal{I}$, that is $\alpha_{A}=2$


## . . . and the bound is tight!

Since $\alpha_{A}$ relates $U B(I)$ and $L B(I), f_{A}(I)$ and $f^{*}(I)$ could be closer Actually, for many instances $\rho_{A}(I)$ is much better than $\alpha_{A}$

Are there instances $\bar{l}$ for which $f_{A}(\bar{I})=\alpha_{A} f^{*}(\bar{I})$ ? How are they like?
The study of these instances is useful to

- evaluate whether they are rare or frequent
- introduce ad hoc modifications to improve the algorithm

In the literature the typical expression "and the bound is tight" introduces the description of instances exhibiting the worst case


If all worst cases are patched, the approximation guarantee improves

## The TSP under the triangle inequality

Consider the TSP with the additional (rather common) assumptions that

- graph $G=(N, A)$ is complete
- $\operatorname{cost} \mathrm{c}$ is nonnegative, symmetric and satisfies the triangle inequality

$$
c_{i j}=c_{j i} \geq 0 \quad \forall i, j \in N \quad \text { and } \quad c_{i j}+c_{j k} \geq c_{i k} \quad \forall i, j, k \in N
$$

Double-tree algorithm
(1) Consider the complete undirected graph corresponding to $G$
(2) Build a minimum cost spanning tree $T^{*}=\left(N, X^{*}\right)$
(3) Make a pre-order visit of $T^{*}$ and build two lists of arcs:
(a) $x^{\prime}$ lists the arcs used both by the visit and the backtracking: this is a circuit visiting each node, possibly several times
(b) $x$ lists the arcs linking the nodes in pre-order ending with the first: this is a circuit visiting each node exactly once

## Example



1) Complete graph $G$ (arcs omitted)

2. Minimum spanning tree $T^{*}$


$$
\text { 3.a) } \begin{array}{r}
x^{\prime}=(A, C, F, H, F, I, F, C, D, G, \\
L, G, E, G, D, B, D, C, A)
\end{array}
$$

$$
\text { 3.b) } x=(A, C, F, H, I, D, G, L, E, B, A)
$$

The double-tree algorithm is 2-approximated
(1) the cost of the minimum spanning tree is an underestimate $L B(I)$

- deleting an arc from a Hamiltonian circuit yields a Hamiltonian path that is cheaper
- a Hamiltonian path is a spanning tree (usually not of minimum cost)
(2) the cost of circuit $x^{\prime}$ is
- an overestimate $U B(I)$ (it is a nonminimum Hamiltonian circuit)
- equal to $2 L B(I)$ (two arcs correspond to each edge)
(3) the cost of circuit $x$ is $f_{A}(I) \leq U B(I)$
(a single direct arc replacing a sequence decreases the cost)
This implies that $f_{A}(I) \leq 2 f^{*}(I)$ for each $I \in \mathcal{I}$, that is $\alpha_{A}=2$
Notice: $x^{\prime}$ is used in the approximation proof, but needs not be computed


## Inapproximability

For an inapproximable problem, approximated algorithms would be exact
Consider this family of TSP instances on complete graphs:

- $c_{i j}=0$ for $(i, j) \in A_{0}$
- $c_{i j}=1$ for $(i, j) \in(N \times N) \backslash A_{0}$ (the triangle inequality is violated!) The optimum of any such instance $\bar{I}$ is:

$$
\left\{\begin{array}{l}
f^{*}(\bar{I})=0 \text { if } A_{0} \text { contains a Hamiltonian circuit } \\
f^{*}(\bar{I}) \geq 1 \text { otherwise }
\end{array}\right.
$$

(in the latter case, the optimal solution contains at least an arc $\notin A_{0}$ )
Assume that a polynomial algorithm $A$ provide a guarantee $\alpha_{A}$

$$
f^{*}(I) \leq f_{A}(I) \leq \alpha_{A} f^{*}(I) \forall I \in \mathcal{I}
$$

Then $f^{*}(\bar{I})=0 \Leftrightarrow f_{A}(\bar{I})=0$
Whenever the subgraph $G\left(N, A_{0}\right)$ has a Hamiltonian circuit, $A$ finds it, solving an $\mathcal{N} \mathcal{P}$-complete problem in polynomial time ( $\mathcal{P}=\mathcal{N} \mathcal{P}$ )

## Approximation schemes

For hard problems

- exact algorithms provide the best approximation guarantee ( $\alpha_{\boldsymbol{A}}=1$ ), but require exponential time $T_{A}$
- approximated algorithms provide a worse guarantee ( $\alpha_{A}>1$ ), but could require polynomial time $T_{A}$

Some problems admit a family of algorithms providing a whole range of compromises between efficiency ed effectiveness

- better and better approximation guarantees: $\alpha_{A_{1}}>\ldots>\alpha_{A_{r}}$
- worse and worse computational complexities: $T_{A_{1}}<\ldots<T_{A_{r}}$

Approximation scheme is a parametric algorithm $A_{\alpha}$ allowing to choose $\alpha$
(Example: the $K P$ )

## Beyond the worst case

As usual, the worst-case approach is rough:
some algorithms often have a good performance, though sometimes bad
The alternative approaches are similar to the ones used for complexity

- parametrisation: prove an approximation guarantee that depends on other parameters of the instances besides the size $n$
- average-case: assume a probability distribution on the instances and evaluate the expected value of the approximation factor (the algorithm could have a bad performance only on rare instances)
but there is at least another approach
- randomisation: the operations of the algorithm depend not only on the instance, but also on pseudorandom numbers, so that the solution becomes a random variable which can be investigated (the time complexity could also be random, but usually is not)


## Randomised approximation algorithms

For a randomised algorithm $A, f_{A}(I, \omega)$ and $\rho_{A}(I, \omega)$ are random variables depending on the pseudorandom number seed $\omega$

A randomised approximation algorithm has an approximation ratio whose expected value is limited by a constant

$$
E\left[\rho_{A}(I, \omega)\right] \leq \alpha_{A} \text { for each } I \in \mathcal{I}
$$

Max-SAT problem: given a CNF, find a truth assignment to the logical variables that satisfy a maximum weight subset of formulae

Purely random algorithm:
Assign to each variable $x_{j}(j=1, \ldots, n)$

- value False with probability $1 / 2$
- value True with probability $1 / 2$

What is the expected value of the solution?

## Randomised approximation for the MAX-SAT

Let $\delta_{i}(x)$ be 1 if solution $x$ satisfies clause $i, 0$ otherwise
The objective $f(x)=f_{A}(I, \omega)$ is the total weight of the satisfied clauses and its expected value is

$$
E\left[f_{A}(I, \omega)\right]=E\left[\sum_{i \in \mathcal{C}} \delta_{i}(x) w_{i}\right]=\sum_{i \in \mathcal{C}}\left(w_{i} \cdot \operatorname{Pr}\left[\delta_{i}(x)=1\right]\right)
$$

Let $k_{i}$ be the number of literals of formula $i \in \mathcal{C}$ and $k_{\text {min }}=\min _{i \in \mathcal{C}} k_{i}$

$$
\begin{aligned}
& \operatorname{Pr}\left[\delta_{i}(x)=1\right]=1-\left(\frac{1}{2}\right)^{k_{i}} \geq 1-\left(\frac{1}{2}\right)^{k_{\min }} \text { for each } i \in \mathcal{C} \\
\Rightarrow & E\left[f_{A}(I, \omega)\right] \geq \sum_{i \in \mathcal{C}} w_{i} \cdot\left[1-\left(\frac{1}{2}\right)^{k_{\min }}\right]=\left[1-\left(\frac{1}{2}\right)^{k_{\min }}\right] \sum_{i \in \mathcal{C}} w_{i}
\end{aligned}
$$

and since $\sum_{i \in \mathcal{C}} w_{i} \geq f^{*}(I)$ for each $I \in \mathcal{I}$ one obtains

$$
\frac{E\left[f_{A}(I, \omega)\right]}{f^{*}(I)} \geq\left[1-\left(\frac{1}{2}\right)^{k_{\min }}\right] \geq \frac{1}{2}
$$

