Introduction to metaheuristics for combinatorial optimization

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Optimization

Goal: Find a solution **satisfying** the constraints and which is **optimal** with respect to a given criterion.

Two problems:

1. Constrained optimization (optimisation sous contraintes): see above
2. **Optimization: just minimize a criterion**

Two big approaches:

1. Complete/exact/guaranteed algorithms
2. **Incomplete/inexact algorithms (heuristics or metaheuristics)**

Objective Function

Definition: the cost function (criterion) to be optimized. The objective function can be evaluated on a complete instantiation.
(An estimate of the objective function can often be given on a partial instantiation.)

Examples of objective functions:

- Scheduling problems: minimizing the due date of the latest task in the problem.
- Resource allocation problems: minimizing the number of resources
- Configuration or design problems: minimizing the price of production
- MAX-CSP: minimizing the number of violated constraints (or a weighted sum of violated constraints)

Contents

Overview

Optimization heuristics work on a **current solution (configuration)**: a point of the search space (actual solution or not).

Neighborhood: the set of configurations which can be obtained by a local transformation of the current configuration. Examples:

- Graph-Coloring: change a color
- SAT: “flip” of one boolean variable
- CSP: modification of one variable value ($n(d-1)$ neighbors)

Evaluation of a configuration: cost of the configuration: value to be minimized during search

Local search: improve a current configuration by iterative local transformations

SAT and CSP models

Definitions

Examples : Sudoku, graph coloring, many industrial problems

Solving the problem by **minimizing** the conflicts in MaxSAT (minimizing the number violated clauses) and MaxCSP (minimizing the number of violated constraints)

Descent algorithm (algo de descente)

Also called *hill climbing* or greedy algorithm

Initial configuration

- random: any point in the search space, or
- given by a deterministic (greedy) algorithm: a not too bad initial point should lead to a good configuration

Local search

While a halt criterion is not fullfilled and a better configuration is found do:

1. Search a better configuration (or the best one) in the neighboring of the current configuration.
2. Change the current configuration to the selected neighbor (if any).

Drawback

The descent algorithm finds a **local optimum**.

Drawbacks of metaheuristics

- **Incompleteness:** the search is not systematic (all the possibilities are not tried) $\Longrightarrow$
  no guarantee that the best solution has been found (no proof of the best solution)
- **Local optimum:** a local search may be blocked within a local optimum.
  It may be blocked on a plateau and sometimes visits several times the same configurations.
- **Sensitivity to the initial configuration**

Several improvements

Most of the following improvements aim at avoiding local minima and plateaus. More generally, they follow the **Intensification/Diversification** mechanism.

- Interrupt the current search and try again with other initial configurations $\Longrightarrow$ **GSAT** (random initial configurations) or other **multi-start** strategies with selected relaunch points.
- Manage several configurations in parallel (a "population" of configurations) $\Longrightarrow$ **genetic algorithms**, **GWW** (and ant and bees metaheuritics).
- Record the latest moves to avoid looping on the same configurations $\Longrightarrow$ **tabu search (TS)**
- Sometimes accept a configuration which gives a worse configuration $\Longrightarrow$ **simulated annealing (SA)**, threshold accepting (TA)
- Use only the neighbors management to intensify or diversify the search: candidate list strategies (CLS), including **IDWalk**.

A generic metaheuristic

Goal: design (and explain) most of existing optimization heuristics
Parameters:

- `Max-Tries`: number of times a local search is performed (from different initial configurations)
- `Max-Moves`: maximum number of steps in every walk
- `Accepted?(x, x': configurations) : boolean`
  The function checking whether the neighbor x' of x is an acceptable move
- `Max-Neighbors`: maximum number of neighbors which are visited for any move
- `Min-Neighbors`: minimum number of neighbors which are visited for any move
- `No-Acceptation`: value taken into account when no neighbor has been accepted (among `Max-Neighbors` ones). Can either be equal to:
  - `no-move`: no new neighbor is selected (and the current walk is stopped)
  - `one-neighbor`: any visited neighbor is selected (e.g. the last one)
  - `best-neighbor`: a “less bad neighbor” is selected

A generic metaheuristic

```
Algorithm GenericMetaheuristic(...)    Returns: a configuration
    best ← $\perp$
    for i=1 to Max-Tries do
        $x$ ← Initial-Configuration(...)
        $j \leftarrow 0$
        best-walk ← $\perp$
        while $j <$ Max-Moves do
            $x$ ← Generic-Move ($x$)
            best-walk ← Minimum(best-walk, $x$)
        end
        best ← Minimum(best, best-walk)
    end
    return best
end.
```

Acceptation of a move

```
Algorithm Generic-Move(init : initial configuration) Returns: final configuration
    $i \leftarrow 0$
    best? ← (Min-Neighbors $> 1$) or (No-Acceptation=best-neighbor)
    best-cost ← $+\infty$ ; x-best ← init ; x ← init ; accepted? ← false
    while ($i <$ Min-Neighbors) or ($i <$ Max-Neighbors and not(accepted?))
    do
        $x' \leftarrow$ Generate-Neighbor($x$)
        if Accepted?($x, x'$) then accepted? ← true
        if best? and (cost($x'$) < best-cost) then
            x-best ← $x'$
            best-cost ← cost($x'$)
        end
        $i \leftarrow i + 1$
    end
    if accepted? then
        if best? then
            return x-best
        else
            return $x'$
        end
    end
    if No-Acceptation=best-neighbor then return x-best
    if No-Acceptation=one-neighbor  then return $x'$
    if No-Acceptation=no-move       then return $x$
end.
```

Simulated Annealing (SA) method

En francais : algorithme du *recuit simulé*
One of the oldest local search algorithms

Deduced from `Generic-Move`:

- `Generate-Neighbor`(x): any neighbor (selected randomly)
- `Min-Neighbors` = number of neighbors (variant: `Min-Neighbors`= `Max-Neighbors`)
- `No-Acceptation` = `no-move` (+ interruption of the walk)
- `Accepted?`(x, x') : `cost`(x') $\leq$ `cost`(x) **or** `Random()` $<$ $\exp(\frac{-\Delta}{T})$

Simulated Annealing (SA) method

```
Algorithm SA-Move(init: initial configuration, T: a temperature,
Min-Neighbors : number of neighbors) Returns: final configuration
    best-cost ← $+\infty$ ; x-best ← init ; x ← init
    $i \leftarrow 0$ ; accepted? ← false
    while ($i <$ Min-Neighbors) do
        $x' \leftarrow$ Generate-Neighbor($x$)
        if cost($x'$) $\leq$ cost($x$) or Random() $< \exp(\frac{-\Delta}{T})$ then
            accepted? ← true
        end
        if cost($x'$) $<$ best-cost then
            x-best ← $x'$
            best-cost ← cost($x'$)
        end
        $i \leftarrow i + 1$
    end
    if accepted? then
        return x-best
    else
        return $x$
    end
end.
```

Simulated Annealing (SA) method

The important parameter is the **temperature** T, inspired from the physical phenomenon of *annealing*:

- Δ represents the degree of deterioration of the criterion, e.g., the additional number of violated constraints in MAX-CSP.
- A high temperature T allows the algorithm to escape from local minima.
- A low temperature makes the algorithm a greedy algorithm.
- The temperature should smoothly decrease (annealing process):
  Theoretical *convergence* with a infinitely smooth decrease.
  Variant: the Metropolis algorithm with a constant temperature.

The Tabu Search (TS) method

Idea: Management of a *tabu list*: list of constant length L which records the L latest moves (FIFO). For CSPs, a move $x' - x$ in the tabu list is the modified variable (the value is not stored). The tabu list avoids looking several times at the same configuration.

Definition:

- `Min-Neighbors` = number of neighbors (variant: `Min-Neighbors`= `Max-Neighbors`)
- `No-Acceptation` = `no-move` (+ interruption of the walk)
- `Accepted?`(x, x', `tabu-list`) : $x' - x \notin$ `tabu-list` or x' has the best cost ever found (*aspiration*).

An important parameter is the length L of the tabu list.
Question: what allows the algorithm to escape from local minima?

The Tabu Search (TS) method

```
Algorithm TS-Move(init: current configuration, in-out tabu-list, L: max length of
tabu list, Min-Neighbor: number of neighbors) Returns: next configuration
    best-cost ← $+\infty$ ; x-best ← init ; x ← init
    $i \leftarrow 0$ ; accepted? ← false
    while ($i <$ Min-Neighbors) do
        $x' \leftarrow$ Generate-Neighbor($x$)
        if $x' - x \notin$ tabu-list or cost($x'$) < best-cost (aspiration) then
            accepted? ← true
        end
        if cost($x'$) < best-cost then
            x-best ← $x'$
            best-cost ← cost($x'$)
        end
        $i \leftarrow i + 1$
    end
    if accepted? then
        tabu-list.PushEnd(x-best)
        if (size(tabu-list) > $L$) then tabu-list.PopFirst()
        return x-best
    else
        return $x$
    end
end.
```

Variants of the Tabu Search

Fred Glover has introduced a lot of mechanisms in the tabu search schema for solving miscellaneous operational research problems. Two variants:

- *Probabilistic tabu*: a probability of acceptance is associated to every neighbor (the sum equals to 1). The value depends on when a move has been pushed in the list, the quality of the neighbor, and so on.
- Dynamic tabu list: the length L of the tabu list is modified in the course of time:
  - L follows a pattern (e.g., a sinosoide) modifying the ratio Intensification vs Diversification during time: *strategic oscillation*.
  - L is *adaptive*, that is, changes according the difficulty to improve the current configuration.

Candidate list strategies and IdWalk

Principle: Take a lot of care in the analysis of the candidates (neighbors) for the next move: encode most of the local search mechanisms (such as Intensification vs Diversification) inside the function **Generic-move**!

Example: the **Intensification Diversification Walk (IDW)** algorithm:
Definition:

- `Accepted?`(x, x') : $x' \leq x$ (greedy component: Intensification)
- `Min-Neighbors` $= 0$
- `No-Acceptation` $=$ `one-move` or `best-move` (random component: Diversification)
- Main parameter to be tuned: `Max-Neighbors` with 3 roles:
  1. limits the number of explored neighbors,
  2. must be sufficiently large for intensifying the search,
  3. must be sufficiently small for diversifying the search (with `No-Acceptation`).

ID Walk

Algorithm IDW-Move(*init: current configuration,* `Max-Neighbor`*: number of neighbors*) **Returns:** *next configuration*

```
    best-cost ← $+\infty$ ; x-best ← $init$ ; x ← $init$
    $i \leftarrow 0$ ; accepted? ← false
    while ($i <$ Max-Neighbors and not(accepted?)) do
        $x' \leftarrow$ Generate-Neighbor($x$)
        if cost($x'$) $\leq$ cost($x$) then
            accepted? ← true
        end
        if cost($x'$) $<$ best-cost then
            x-best ← $x'$
            best-cost ← cost($x'$)
        end
        $i \leftarrow i + 1$
    end
    if accepted? then
        return $x'$
    else
        return x-best /* Variant: return $x'$ */
    end
end.
```

Genetic algorithms: guidelines

Management of a **population** of configurations, called **individuals**

```
Algorithm GA-schema
    while no satisfactory individuals in the population do
        Select individuals in the population for reproduction
        Apply different reproduction operators on selected
        individuals:
            • mutation: generation of a neighbor of an individual
            • crossover: mixing two configurations (individuals)
              to generate a new individual
    end
    Selection: keep a sub-set of the new population
    (natural selection)
end.
```

Encoding: an individual is made of a chromosom: a sequence of bits

Another population algorithm: Go With the Winners

`GWW` manages several configurations (called *particles*) and a threshold (in French: seuil).

Initialization: *B* particules are randomly distributed; a threshold is placed at the cost of the worst particle.

Main loop: `repeat until` *no particle remains under or at the threshold*:

1. **Redistribution:** (bad) particules over the threshold are “redistributed”: a redistributed particle is replaced by a copy of another particle (under the threshold; randomly chosen).
2. **Randomization:** A random walk of length *S* is performed: every step of the walk moves a particle to a neighbor *which remains at or under the threshold*.
3. Lower the threshold value by 1.

Genetic Algorithms for (MAX-)CSP

The population is a set of configurations.

Evaluation function of an individual: number of conflicts, weighted sum of conflicts...

Difficulty: the crossover operator is not relevant
$\Longrightarrow$ difficult to generate a better individual.

- The crossover point does not take the number of conflicts into account.
- A chromosom loses the topology of the constraint system (This drawback is also true for most of the non-structured combinatorial problems.)

Heuristic reparation by Minton (for CSPs)

Initialization: greedy instantiation of variables: iteratively choose the variable which produces a smallest number of conflicts with previous variables.

Reparation: `While` *there is a conflict* `do`:

- choose a variable x whose value gives at least one conflict
- change the value of x to a new value which minimizes the number of conflicts

`Min-Neighbors`? `No-Acceptation`
? `best-neighbor`? `Accepted?` ? ...?

GSAT

Initially developed for SAT (satisfiability of a boolean formula)

Definition: several trials of the descent algorithm

- Neighborhood: the *n* configurations where a single variable is "flipped".
- `Max-Tries` $>> 1$
- `Max-Moves` is limited
- `Max-Neighbors` = number of neighbors
- `Min-Neighbors` = `Max-Neighbors`
- `No-Acceptation` = `best-move`
  (or `no-move` + interruption of the walk)
- `Accepted?`(x, x') : `cost`$(x') \leq$ `cost`(x)

`Max-Tries` allows GSAT to find several local minima, one being maybe a global minimum

WalkSAT (for SAT)

Choose an **unsatisfied** clause C
(Flipping any variable in C will at least fix C)

Compute a “break score”: for each var v in C, flipping v would break how many other clauses?

1. If C has any vars with break score 0:
   Pick at random among the vars with break score 0
2. else, with probability p:
   - Pick at random among the variables with minimum break score
   - else: Pick at random among all variables in C (large diversification)

Example of experiments

le15c, le25c and flat28 are graph coloring instances (encoded as MAX-CSP instances); celar6, celar7, celar8 are radio link frequency assignment instances.

An entry contains the average cost (over 10 or 20 trials). The best cost over the 10 or 20 trials appears into parentheses.

The neighborhood definition is crucial! (not detailed here)

	le15c	**le25c**	**flat28**	**celar6**	**celar7**	**celar8**
# colors	15	25	31			
Time/trial	2 min	14 min	9 min	14 min	6 min	50 min
Metrop.	5.9 (2)	**3.1** (2)	0.9 **(0)**	5048 (3906)	$6\,10^6$ ($2.9\,10^6$)	410 (300)
SA	9.6 **(0)**	5.8 (4)	1.8 **(0)**	4167 (3539)	$1.2\,10^6$ (456893)	281 (264)
Tabu	1.5 **(0)**	3.7 (3)	2.5 (1)	4183 (3935)	$1.2\,10^6$ (620159)	373 (315)
IDWalk	0.5 **(0)**	**3.1 (1)**	**0.8 (0)**	3447 **(3389)**	373334 (343998)	291 (273)
GWW	536 (410)	17.1 (14)	6.6 (6)	3648 (3427)	583278 (456968)	276 (265)
GWW-idw	**0 (0)**	4 (3)	1.3 **(0)**	**3405 (3389)**	**368452 (343600)**	**267 (262)**

Synthesis

Optimization heuristics are incomplete, but are less sensitive to bad choices than exact methods.

What is important if one wants to find, with local search, a good solution to a given optimizatiom problem:

1. Try several ways of encoding the problem (definition of neighboring).
2. Understand the intuitions (i.e., the useful mechanisms) behind the main optimization heuristics.
3. Be pragmatic, have no strong belief: Try different heuristics, instead of tuning only one: use a library!
4. Favor the simplest ideas because they are faster to understand and experiment.
5. A fine tuning of the parameters generally does not pay.
6. Favor adaptive parameters.