Heuristic Algorithms

Master's Degree in Computer Science/Mathematics

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Genetic algorithms

Algorithm GeneticAlgorithm$(I, X^{(0)})$

$\Xi^{(0)} := Encode(X^{(0)})$; $x^* := \arg\min_{x \in X^{(0)}} f(x)$; { Best solution found so far }

For $g = 1$ *to* n_g *do*

$\Xi := Selection(\Xi)$;

$\Xi := Crossover(\Xi)$;

$x_c := \arg\min_{\xi \in \Xi} f(x(\xi))$;

If $f(x_c) < f(x^*)$ *then* $x^* := x_c$;

$\Xi := Mutation(\Xi)$;

$x_m := \arg\min_{\xi \in \Xi} f(x(\xi))$;

If $f(x_m) < f(x^*)$ *then* $x^* := x_m$;

EndFor;

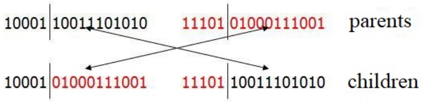
Return $(x^*, f(x^*))$;

Crossover

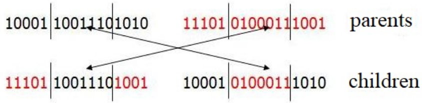
The crossover operator combines $k \geq 2$ individuals to generate other k

The most common ones set $k = 2$ and are

- simple crossover:
  - extract a random position with uniform probability
  - split the encoding in two parts at the extracted position
  - exchange the final parts of the encodings of the two individuals



- double crossover:
  - extract two positions at random with uniform probability
  - split the encoding in three parts at the extracted positions
  - exchange the extreme parts of the encodings of the two individuals



Crossover

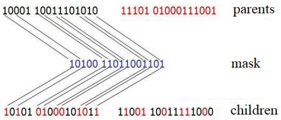
Generalizing, one obtains the

- α points crossover:
  - extract α positions at random with uniform probability
  - split the encoding in $\alpha + 1$ parts at the extracted positions
  - exchange the odd parts of the encodings of the two individuals (first, third, etc...)

For small values of α, this implies a positional bias:
symbols close in the encoding tend to remain close

To cancel this bias, one can adopt the

- uniform crossover:
  - build a random binary vector $m \in U(\mathbb{B}^n)$ ("mask")
  - if $m_i = 1$ exchange the symbols in position i of the two individuals, if $m_i = 0$ keep them unmodified



Crossover versus Scatter Search and Path Relinking

The crossover operator resembles the recombination phase of *SS* and *PR*

The main differences are that

1. it recombines the symbols of the encodings, instead of
   - recombining the solutions (*SS*)
   - performing a chain of exchanges on the solutions (*PR*)
2. it operates on the whole population, instead of only a reference set R
3. it operates on random pairs of individuals, instead of methodically scanning all pairs of solutions of R
4. it generates a pair of new individuals, instead of
   - generating a single intermediate solution (*SS*)
   - visiting the intermediate solutions and choosing the best one (*PR*)
5. the new individuals enter the population directly, instead of becoming candidates for the reference set

However, classifying an operator can be a matter of taste

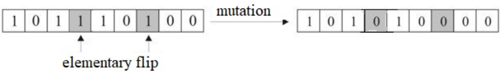
Mutation

The mutation operator modifies an individual to generate a similar one

- scan encoding ξ one symbol at a time
- decide with probability π_m to modify the current symbol

The kind of modification usually depends on the encoding

- binary encodings: flip ξ_i into $\xi_i' := 1 - \xi_1$



- symbol strings: replace ξ_c with a random symbol $\xi_c' \in B_c \setminus \{\xi_c\}$ selected with a uniform probability
- permutations: there are many proposals
  - exchange two random elements in the permutation (*swap*)
  - reverse the stretch between two random positions of the permutation
  - ...

Mutation versus exchange heuristics

The mutation operator has strong relations with exchange operations

The main differences are that

1. it modifies the symbols of an encoding,
   instead of exchanging elements of a solution
2. it operates on random symbols,
   instead of exploring a neighbourhood systematically
3. it operates on a random subset of symbols of size unknown *a priori*,
   somewhat like sampling a very large scale neighbourhood,
   instead of exchanging a fixed number of elements
4. it operates on random individuals, instead of all solutions
5. the new individuals enter the population directly,
   instead of becoming candidates for the reference set

However, classifying an operator can be a matter of taste

The feasibility problem

If the encoding is not fully invertible, crossover and mutations sometimes generate encodings that do not correspond to feasible solutions

We distinguish between

- feasible encodings that correspond to feasible solutions
- unfeasible encodings that correspond to legal, but unfeasible subsets

The existence of unfeasible encodings implies several disadvantages:

- inefficiency: computational time is lost handling meaningless objects
- ineffectiveness: the heuristic explores less solutions (possibly, none)
- design problems: fitness must be defined also on unfeasible subsets

There are three main approaches to face this problem

1. special encodings and operators (*avoid or limit infeasibility*)
2. repair procedures (*turn infeasibility into feasibility*)
3. penalty functions (*accept infeasibility, but discourage it*)

Special encodings and operators

The idea is to investigate

- encodings that (nearly) always yield feasible solutions, such as
  - permutation encodings and order-first split-second decodings for partition problems (*CMSTP*, *VRP*, etc...)
  - permutation encodings and constructive heuristic decodings for scheduling problems (*PMSP*,...)
- crossover and mutation operators that maintain feasibility, such as
  - operators that simulate moves on solutions (k-exchanges)
  - specialised operators (*Order* or *PMX* crossover for the *TSP*)

These methods

- tend to closely approximate exchange and recombination heuristics based on the concept of neighbourhood
- give up the idea of abstraction and focus on the specific problem, contrary to classical genetic algorithms

Repair procedures

A repair procedure is a refined decoder function $x_R : \Xi \to X$ that

- decodes any encoding ξ into a possibly unfeasible solution $x(\xi) \notin X$
- transforms subset $x(\xi)$ into a feasible solution $x_R(\xi) \in X$
- returns x_R

The procedure is applied to each unfeasible encoding $\xi \in \Xi^{(g)}$

- in some methods, the encoding $\xi(x_R(\xi))$ replaces ξ in $X^{(g)}$
- in other ones, ξ remains in $\Xi^{(g)}$ and $x_R(\xi)$ is used only to update x^*

The methods of the first family

- maintain a population of feasible solutions

but they introduce

- a strong bias in favour of feasible encodings
- a bias in favour of the feasible solutions most easily obtained with the repair procedure

Penalty functions: measuring the infeasibility

If the objective function is extended to unfeasible subsets $x \in 2^B \setminus X$, the fitness function $\phi(\xi)$ can be extended to any encoding, but many unfeasible subsets have a fitness larger than the optimal solution

The selection operator tends to favour such unfeasible subsets

To avoid that, the fitness function must combine

- the objective value $f(x(\xi))$
- a measure of infeasibility $\psi(x(\xi))$

$$\begin{cases} \psi(x(\xi)) = 0 \text{ if } x(\xi) \in X \\ \psi(x(\xi)) > 0 \text{ if } x(\xi) \notin X \end{cases}$$

If the constraints of the problem are espressed by equalities or inequalities, $\psi(x)$ can be defined as a weighted sum of their violations

How to define the weights?
Are they fixed, variable or adaptive?

Penalty functions: definition of the fitness

The most typical combinations are

- absolute penalty: minimise ψ and f lexicographically;
  given two encodings ξ and ξ' in a rank or tournament selection
  - choose the less unfeasible one
  - if they are equally (un)feasible, choose the better
- proportional penalty: use a linear combination of f and ψ

  $$\varphi(\xi) = f(x(\xi)) - \alpha\psi(x(\xi)) + M \qquad \text{for maximisation problems}$$

  $$\varphi(\xi) = -f(x(\xi)) - \alpha\psi(x(\xi)) + M \qquad \text{for minimisation problems}$$

  where offset M guarantees that $\varphi(\xi) \geq 0$ for all encodings
- penalty obtained by repair, that is keep the unfeasible encoding, but derive its fitness from the objective value of the repaired solution

  $$\varphi(\xi) = f(x_R(\xi)) \text{ or } \varphi(\xi) = UB - f(x_R(\xi))$$

  since usually $f(x_R(\xi))$ is worse than $f(x(\xi))$

Proportional penalty functions: weight tuning

Experimentally, it is better to use the smallest effective penalty

- if the penalty is too small, too few feasible solutions are found
- if the penalty is too large, the search is confined within a part of the feasible region (*"hidden" feasible solutions are hard to find*)

A good value of the parameter α tuning the penalty can be found with

- dynamic methods: increase α over time according to a fixed scheme (*first reach good subsets, then enforce feasibility*)
- adaptive methods: update α depending on the situation
  - increase α when unfeasible encodings dominate the population
  - decrease α when feasible encodings dominate
- evolutionary methods: encode α in each individual, in order to select and refine both the solution and the algorithm parameter

Memetic algorithms

Memetic algorithms (Moscato, 1989) are inspired by the concept of meme (Dawkins, 1976) that is a basic unit of reproducible cultural information

- genes are selected only at the phenotypic expression level
- memes also adapt directly, as in Lamarckian evolution

Out of the metaphor, memetic algorithms combine

- "genotypic" operators that manipulate the encodings (crossover and mutation)
- "phenotypic" operators that manipulate the solutions (local search)

In short, the solutions are improved with exchanges before reencoding

Several parameters determine how to apply local search

- how often (at every generation, or after a sufficient diversification)
- to which individuals (all, the best ones, the most diversified ones)
- for how long (until a local optimum, beyond, or stopping before)
- with what method (steepest descent, VNS, ILS, etc. . .)

Evolution strategies

They have been proposed by Rechenberg and Schwefel (1971)

The main differences with respect to classical genetic algorithms are:

- the solutions are encoded into real vectors
- a small population of μ individuals generate λ candidate descendants (*originally*, $\mu = 1$)
- the new individuals compete to build the new population
  - in the (μ, λ) strategy the best μ descendants replace the original population, even if some are dominated
  - in the $(\mu + \lambda)$ strategy the best μ individuals overall (predecessors or descendants) survive in the new population
- the mutation operator sums to the encoding a random noise with a normal distribution of zero average

$$\xi' := \xi + \delta \text{ with } \delta \in N(0, \sigma)$$

- originally, the crossover operator was not used (*now it is*)

The random-key genetic algorithm (Bean, 1994) use real-vector encodings and decode procedures based on sorting the real numbers