Evolutionary Algorithms

Meta heuristics

and related optimization techniques II/II

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Outline

Swarm- and Population-Based Optimization

swarm intelligence

- part of AI's developing intelligent multi-agent systems
- inspired by the behaviour of certain species, in particular
  - social insects (e.g. ants, termites, bees etc.) and
  - animals living in swarms (e.g. fish, birds etc.)

these species are capable of solving complex tasks by cooperation.

main idea

- generally quite simple individuals with limited skills
- self-coordinated without central control unit
- individuals exchanging information (cooperation)

techniques are classified by their way of information exchange

Techniques

Genetic/Evolutionary Algorithms

- biological pattern: evolution of life
- exchange of information by recombination of genotypes
- every individual serves as a candidate solution

Population Based Incremental Learning

- biological pattern: evolution of life
- exchange of information by prevalence in population
- every individual serves as a candidate solution

Techniques

Particle Swarm Optimization

- biological pattern: foraging of fish or bird swarms for food
- exchange of information by aggregation of single solutions
- every individual serves as a candidate solution

Ant Colony Optimization

- biological pattern: ants searching a route for food
- exchange of information by manipulating their environments (stigmergy, extended phenotype to Darwin)
- individuals generate a candidate solution

Population based incremental learning (PBIL)

- genetic algorithm without population
- instead: only store population statistics ⇒ by $\mathcal{G} = \{0, 1\}^L$ for all L bits the frequency of „1“
- specific individuals (e.g. for evaluation) are generated randomly according to the statistical frequency
- recombination: uniform crossover ⇒ implicitly when generating an individual
- selection: choosing the best individuals B for updating the population statistics $Pr_k^{(t)} \leftarrow B_k \cdot \alpha + Pr_k^{(t-1)}(1 - \alpha)$
- mutation: bit-flipping ⇒ slightly random changes within the population statistics

Algorithm 1 PBIL

Input: evaluation function F
Output: best individual A_{best}

$t \leftarrow 0$
$A_{\text{best}} \leftarrow$ create random individual from $\mathcal{G} = \{0, 1\}^L$
$Pr^{(t)} \leftarrow (0.5, \ldots, 0.5) \in [0, 1]^L$
while termination condition not satisfied {
    $P \leftarrow \emptyset$
    for $i \leftarrow 1, \ldots, \lambda$ {
        $A \leftarrow$ generate individual from $\{0, 1\}^L$ according to $Pr^{(t)}$
        $P \leftarrow P \cup \{A\}$
    }
    evaluate P according to F
    $B \leftarrow$ select best individuals P
    if $F(B) \succ F(A_{\text{best}})$ {
        $A_{\text{best}} \leftarrow B$
    }
    $t \leftarrow t + 1$
    for each $k \in \{1, \ldots, L\}$ {
        $Pr_k^{(t)} \leftarrow B_k \cdot \alpha + Pr_k^{(t-1)}(1 - \alpha)$
    }
    for each $k \in \{1, \ldots, L\}$ {
        $u \leftarrow$ draw a random number according to $U((0, 1])$
        if $u < p_m$ {
            $u' \leftarrow$ draw a random number according to $U(\{0, 1\})$
            $Pr_k^{(t)} \leftarrow u' \cdot \beta + Pr_k^{(t)}(1 - \beta)$
        }
    }
}
return A_{best}

PBIL: Typical Parameters

learning rate α

- low: emphasizes exploration
- high: emphasizes fine tunig

parameter	co-domain
population size λ	20–100
learning rate α	0.05–0.2
mutation rate p_m	0.001–0.02
mutation constant β	0.05

PBIL: Problemes

- algorithm might learn depencencies between certain single bits
- PBIL considers single bits isolated of each other

example:

population 1					population 2			
1	1	0	0	individual 1	1	0	1	0
1	1	0	0	individual 2	0	1	1	0
0	0	1	1	individual 3	0	1	0	1
0	0	1	1	individual 4	1	0	0	1
0.5	0.5	0.5	0.5	population statistics	0.5	0.5	0.5	0.5

- same population statistics can represent different populations

PBIL: Alternatives

- better techniques for estimating the distribution of beneficial candidate solutions
- especially: modelling of internal dependencies (i.e. with bayesian networks)
- example: *Bayesian optimization algorithm (BOA)*
  - create initial population randomly
  - update population for a given number of iterations by applying selection and variation
  - perform selection as usual
  - for variation, apply Bayesian Network as a model of promising candidate solutions
  - create new candidate solutions by reproducing samples from the Bayesian Network

Particle Swarm Optimization

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- fish or birds are searching for rich food resources in swarms
- orientation based on individual search (cognitive part) and other individuals close to them within the swarm (social part)
- also: living within a swarm reduces the risk of getting eaten by a predator

Particle Swarm Optimization

Particle Swarm Optimization [Kennedy and Eberhart, 1995]

- **motivation:** behaviour of swarms of fish (e.g.) when searching for food: randomly swarming out, but always returning to the swarm to exchange information with the other individuals
- **approach:** use a "swarm" of m candidate solutions instead of single ones
- **preconditions:** $\Omega \subseteq \mathbb{R}^n$ and thus the function f $f : \mathbb{R}^n \to \mathbb{R}$ to be maximized (w.l.o.g.)
- **procedure:** take every candidate solution as a "particle" searching for food at the position $\boldsymbol{x}_i$ with a velocity of $\boldsymbol{v}_i$. $(i = 1, \ldots, m)$

⇒ combine elements of ground-oriented search (e.g. gradient descent approach) and population-based search (e.g. EA)

Particle Swarm Optimization

update for position and velocity of particle i:

$$\mathbf{v}_i(t+1) = \alpha \mathbf{v}_i(t) + \beta_1 \left(\mathbf{x}_i^{(\text{local})}(t) - \mathbf{x}_i(t) \right) + \beta_2 \left(\mathbf{x}^{(\text{global})}(t) - \mathbf{x}_i(t) \right)$$

$$\mathbf{x}_i(t+1) = \mathbf{x}_i(t) + \mathbf{v}_i(t)$$

- parameter: β_1, β_2 randomly for every step, α decreasing with t
- $\mathbf{x}_i^{(\text{local})}$ is **local memory** of an individual (particle): the best coordinates being visited by this individual within the search space, i.e.
$$\mathbf{x}_i^{(\text{local})} = \mathbf{x}_i \left(\arg\max_{u=1}^{t} f(\mathbf{x}_i(u)) \right)$$
- $\mathbf{x}^{(\text{global})}$ is **global memory** of the swarm: the best coordinates being visited by any individual of the swarm within the search space (best solution so far), i.e.
$$\mathbf{x}^{(\text{global})}(t) = \mathbf{x}_j^{(\text{local})}(t) \quad \text{mit} \quad j = \arg\max_{i=1}^{m} f\left(\mathbf{x}_i^{(\text{local})} \right)$$

Algorithm 2 Particle swarm optimization

for each particle i $\{$
  $\boldsymbol{x}_i \leftarrow$ choose randomly within search space Ω
  $\boldsymbol{v}_i \leftarrow 0$
$\}$
do $\{$
  for each particle i $\{$
    $y \leftarrow f(\boldsymbol{x}_i)$
    if $y \geq f\left(\boldsymbol{x}_i^{(\text{local})}\right)$ $\{$
      $\boldsymbol{x}_i^{(\text{local})} \leftarrow \boldsymbol{x}_i$
    $\}$
    if $y \geq f\left(\boldsymbol{x}_i^{(\text{global})}\right)$ $\{$
      $\boldsymbol{x}^{(\text{global})} \leftarrow \boldsymbol{x}_i$
    $\}$
  $\}$
  for each particle i $\{$
    $\boldsymbol{v}_i(t+1) \leftarrow \alpha \cdot \boldsymbol{v}_i(t) + \beta_1 \left(\boldsymbol{x}_i^{(\text{local})}(t) - \boldsymbol{x}_i(t)\right) + \beta_2 \left(\boldsymbol{x}^{(\text{global})}(t) - \boldsymbol{x}_i(t)\right)$
    $\boldsymbol{x}_i(t+1) \leftarrow \boldsymbol{x}_i(t) + \boldsymbol{v}_i(t)$
  $\}$
$\}$ **while** termination condition is not satisfied

Extensions

- **reduced search space:** if Ω is a proper subset of $\mathbb{R}^n$ (e.g. hypercube $[a, b]^n$), then all particles will be reflected and bounce off the boundaries of the search space
- **local environment of a particle:** use best local memory of a single particle instead of global swarm memory, e.g. particles surrounding the currently updated one
- **automatic parameter adjustment:** e.g. changing the swarm size (particles being much worse than the currently updated one are extinguished)
- **diversity control:** prevent early convergence to suboptimal solutions e.g. by introducing a new random number for updating the speed to increase diversity

Ant Colony Optimization

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- since food has to be fetched from its source and carried to the nest, ants form transportation roads
- to do this, they label all their routes with scents (pheromones) for other ants may then trace their routes
- this way, routes to food sources are minimized

Ant Colony Optimization

Ant Colony Optimization [Dorigo and Stützle, 2004]

motivation: some ant species are able to find shortest route to food sources by placing and tracing pheromones (scents)

- intuitively: short routes are labeled with more pheromone during the same time
- routes are randomly chosen according to the current pheromone distribution: the more pheromone there is, the more probable is it for ants to choose this way
- the amount of pheromone might vary according to the quality and amount of food found

main principle: stigmergy

- ants are communicating implicitly by placing pheromones
- stigmergy (indirect communication by changing the environmental circumstances) allows for globally adapted behaviour due to locally found information

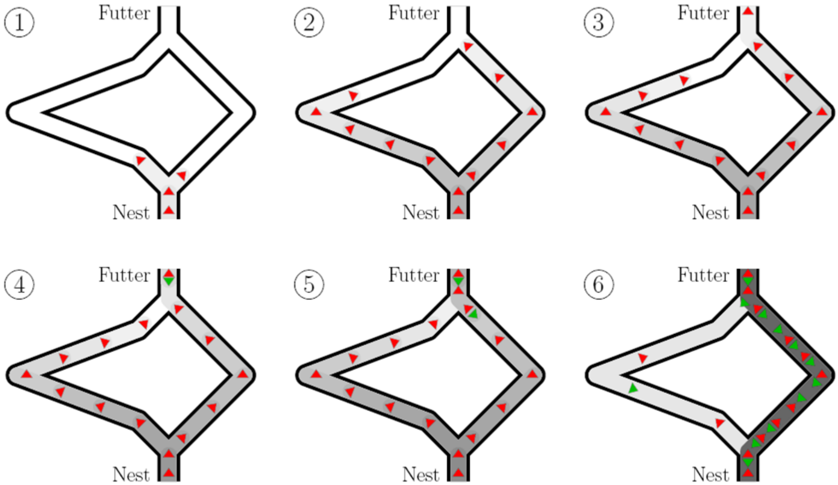
Double-Bridge Experiment [Goss et al., 1989]

- ant nest and food source are connected by 2 bridges that differ in length
- experiment has been run with Argentinian Ants *Iridomyrmex Humilis*: these ants are almost blind (as most other ants, too) so they can't "see" which bridge is shorter
- in most runs: after just several minutes most ants were using the shorter bridge

explanation

- ants travelling the shorter bridge are reaching the food earlier so in the first place the end of the shorter bridge gets more pheromon
- when returning to the nest, choosing the shorter bridge again is more probable for it is labeled with more pheromone now, thus increasing the difference in pheromone even more

Double-Bridge Experiment



Double-Bridge Experiment: Principle

- shorter route is intensified automatically (autocalysis): more pheromon $\longleftrightarrow$ more ants will choose this route
- note: ants are able to find shortest path only because they return on it while placing pheromons again
- when only placing pheromons while running **towards** the food source:
  - at the nest there is no way to decide between both paths as there is no difference in pheromone
  - at the junction of both bridges the ration decreases slowly and finally disappears.
  - by random fluctuation of pheromons the choice for a route might converge towards one of both bridges anyway, but randomly!
- analog (symmetrical situation), if pheromons are only place when returning

Double-Bridge Experiment

- **note:** shorter route is found because of both bridges being available in the very beginning, and not differing in their amount of pheromone
- end of the shorter bridge is reached earlier

$\Rightarrow$ different amount of pheromone on both bridges
$\Rightarrow$ self-intensifying process

- **questions:** What if a new even shorter route is added later by changing the environment?
- Will the ants change for the new route?

answer: No! [Goss et al., 1989]

- once a solution route has been established, the ants will stick to it
- proof: by a second bridge experiment: initializing the experiment with only one (longer) path), later adding a second (shorter) one
- most ants go on using the longer path, only few ants change.

Natural and Artificial Ants

reduce the problem to a search for the best path within a weighted graph

- **problem:** self-intensifying cycles (being visited by an ant a cycle becomes even more probable to be again visited by an ant)
- **solution:** labelling routes only after the ant has completed it's whole tour (thus cycles may be removed from the path)
- **problem:** early convergence to a candidate solution found in the very beginning
- **solution:** pheromone evaporation (not of importance in nature)

useful extensions/improvements

- amount of pheromone dependent on the quality of the solution
- considering heuristics when choosing graph edges (e.g. their weights)

Ant Colony Optimization

- **preconditions:** combinatorial optimization problem with constructive method for creating a solution candidate
- **procedure:** solutions are constructed according to a sequence of random choices, where every choice extends a partial solution
- sequence of choices = path in a decision graph (or construction graph)
- ants ought to explore the paths through a decision graph and find the best (shortest, cheapest) one
- ants label the graph edges with pheromone ⇒ other ants will be guided towards promising solutions
- pheromone “evaporates“ after every iteration so once placed it won’t affect the system for too long (“forgetting“ outdated information)

Application to the TSP

- represent the problem by $n \times n$ matrix $\mathbf{D} = (d_{ij})_{1 \leq i,j \leq n}$
- n cities with distances d_{ij} between city i and j
- note: $\mathbf{D}$ may be asymmetrical, but $\forall i \in \{1, \ldots, n\} : d_{ii} = 0$
- pheromone information as $n \times n$ matrix $\Phi = (\phi_{ij})_{1 \leq i,j \leq n}$
- pheromone value $\phi_{ij} (i \neq j)$ indicates the desirability of visiting city j directly after visiting city i (ϕ_{ii} not used)
- there is no need in keeping Φ symmetrical
- initialize all ϕ_{ij} with the same small value (same amount of pheromone on all edges in the beginning)
- ants run Hamilton tour by labelling the edges of the Hamilton tour with pheromone (with the added pheromone value corresponding to the quality of the found solution)

Constructing a solution

- every ant possesses a “memory“ C where indices of not-yet visited cities are stored
- every visited city is removed from the set C
- there is no such memory in the nature!

1. ant is put randomly to a city where it begins its cycle
2. ant chooses not-yet visited city and goes there: in city i an ant chooses a (not-yet visited) city j with a probability of

$$p_{ij} = \frac{\phi_{ij}}{\sum_{k \in C} \phi_{ik}}.$$

3. repeat step 2 until every city has been visited

Updating the pheromone

1. **evaporation**
   all ϕ_{ij} are reduced by a fraction η (evaporation):
   $$\forall i, j \in \{1, \dots, n\} : \phi_{ij} = (1 - \eta) \cdot \phi_{ij}$$
2. **intensifying a constructed solution:**
   pheromone is put on all edges of the constructed solution corresponding to it's quality::
   $$\forall \pi \in \Pi_t : \phi_{\pi(i)\pi((i \bmod n)+1)} = \phi_{\pi(i)\pi((i \bmod n)+1)} + Q(\pi)$$
   Π_t is the amount used for the tour (permutation) constructed during step t, function of quality: e.g. inverse travelling length
   $$Q(\pi) = c \cdot \left(\sum_{i=i}^{n} d_{\pi(i)\pi((i \bmod n)+1)} \right)^{-1}$$
   „The better the solution, the more pheromone is added.“

Travelling Salesman Problem

Algorithm 3 Ant colony optimization for TSP

initialize all elements ϕ_{ij}, $1 \leq i, j \leq n$ of the matrix, with small ϵ
do {
  for each Ant { /* generate candidate solution */
    $C \leftarrow \{1, \ldots, n\}$ /* set of cities to be visited */
    $i \leftarrow$ draw a hometown randomly from C
    $C \leftarrow C \setminus \{i\}$ /* remove it from the set of not-yet visited cities */
    while $C \neq \emptyset$ { /* while there are not-yet visited cities */
      $j \leftarrow$ draw the next city from C with probability p_{ij}
      $C \leftarrow C \setminus \{j\}$ /* remove it from the set of not-yet visited cities */
      $i \leftarrow j$ /* and move there */.
    }
  }
  update matrix of pheromones Φ according to the fitness of the solution
} **while** termination condition is not satisfied

Extensions and Alternatives

- **prefer nearby cities:** (analogical to next neighbor heuristics)
  move from city i to city j with probability

$$p_{ij} = \frac{\phi_{ij}^{\alpha}\tau_{ij}^{\beta}}{\sum_{k \in C} \phi_{ik}^{\alpha}\tau_{ik}^{\beta}}$$

  with C = set of indices of not-yet visited cities and $\tau_{ij} = d_{ij}^{-1}$
- **tend to choosing the best edge:** (greedy)
  with probability p_{exploit} move from city i to city j_{best} with

$$j_{\text{best}} = \arg\max_{j \in C} \phi_{ij} \quad \text{bzw.} \quad j_{\text{best}} = \arg\max_{j \in C} \phi_{ij}^{\alpha}\tau_{ij}^{\beta}$$

  and use p_{ij} with probability $1 - p_{\text{exploit}}$
- **intensify best known tour:** (elitism)
  label it with extra pheromone (e.g. the fraction of additional ants that pass it)

Extensions and Alternatives

ranking based updates

- place pheromone only on edges of last iteration's best solution (and possibly on the best overall solution, too)
- amount of pheromone depends on the rank of the solution

strict elite principles

- place pheromone only on the last iteration's best solution
- place pheromone only on the best solution found so far

Extensions and Alternatives

minimal/maximal amount of pheromone

- set an upper or lower limit of pheromone for the edges

⇒ sets an upper or lower limit for the probability of choosing an edge

⇒ better search space exploration, but might lead to worse convergence

limited evaporation

- pheromone evaporates only on edges, that have been used during this iteration

⇒ better search space exploration

Improving a tour locally

- considering local improvements of a candidate solution is promising: Before updating the pheromone the generated tour is optimized locally. (simple modifications are checked for giving benefit)
- local optimizations include e.g.:
  - **recombination after removing 2 edges** (2-opt) can be seen as “reversing“ a part of a tour
  - **recombination after removing 3 edges** (3-opt) can be seen as “reversing“ two parts of a tour
  - **limited recombination** (2.5-opt)
  - **exchanging neighboring cities**
  - **permutation of neighboring city-triplets**
- apply „expensive“ local optimization only to the best solution found so far (or found during the last iteration)

General Application to Optimization Problems

- **general idea**
  consider the problem as searching a (decision) graph, with the candidate solutions being described by sets of edges (note: these sets are not required to form paths!)

- **general description:** for each problem below we describe
  - nodes and edges of the decision/construction graph
  - constraints
  - significance of the pheromone on edges (and possibly nodes)
  - useful heuristics
  - generation of a candidate solution

- the algorithmic approach is similar to those used for TSP

General Application to Optimization Problems: TSP

- *nodes and edges of the decision/construction graph*: the cities to be visited, and their weighted connections (weights being distance, time, costs)
- *constraints:* visit every city exactly once
- *meaning of pheromone on the edges:* the desirability of visiting city j right after city i
- *useful heuristics:* distances between the cities, prefer close cities
- *generation of a solution candidate:* starting at a randomly chosen city always progress to another, not-yet visited city

General Application to Optimization Problems

General Assignment Problem

assign n tasks to m working units (workmen/machines): minimizing the sum of assignment costs d_{ij} with respect to the maximal capacity ρ_j for given capacity costs r_{ij}, $1 \leq i \leq n$, $1 \leq j \leq m$

- every task and every working unit = node of the construction graph (edges are labled with the costs of assignment d_{ij})
- every task has to be assigned to exactly one working unit without exceeding their capacity
- pheromones upon the edges are used for describing the desirability of assigning a task to a working unit
- inverse absolute or relative r_{ij} oder inverse d_{ij}
- choose edges step by step, not necessarily creating a path. Skip edges of tasks that have already been assigned (penalize candidate solutions that violate constraints (e.g. by raising costs))

General Application to Optimization Problems

Knapsack Problem

Choose a subset of maximal value from a set of n objects with a value of w_i, a weight of g_i, a volume of v_i, etc. $1 \leq i \leq n$ with respect to an upper limit for weight, volume etc.

- every object = node within the construction graph, labeled with their value w_i. Edges are not needed
- upper limit for weight, volume etc. has to be respected
- pheromone: assigned only to nodes, describing the desirability of choosing the corresponding object
- ratio between an object and it's relative weight, volume etc. if necessary with respect to the limits
- choose nodes step by step whilst making sure to not exceed the limits

Convergence of the Search

consider "standard behaviour" with the following attributes:

- pheromone evaporating on all edges with a constant factor
- placing pheromone only on the best candidate solution found so far (strict elite principle)
- $\exists$ lower bound $\phi_{\min}$ for pheromone amount on the edges, which is not to be exceeded

- standard procedure converges in probability towards a solution, i.e. the probability for finding a solution goes to 1 with $t \to \infty$

- when the lower bound $\phi_{\min}$ for pheromone values is approaching 0 "sufficiently slow" ($\phi_{\min} = \frac{c}{\ln(t+1)}$ with a number of increments t and a constant c), it can be shown that for $t \to \infty$ the probability for every ant generating a solution will approach 1.

Summary

- swarm and population based algorithms: **heuristics for solving optimization problems**
- purpose: finding a good approximation of the solution
- attempt to reduce the **problem of local optima** (by improving exploration of the search space)
- important: **exchange of information** between individuals (depending on the principle: different types of algorithms)
- **particle swarm optimization**
  - optimization of a function with real agruments
  - exchange of information by watching the neighbors
- **ant colony optimization**
  - search for best routes (abstract: within a decision graph)
  - exchange of information: manipulation of the environment (stigmergy)

Outline

1. Swarm- And Population-Based Optimization

2. Organic Computing

3. Summary

Motivation

In the future independent systems will

- be able to communicate,
- adapt to their environment automatically,
- be used in many different fields.

Examples for such systems:

- administration of peer-to-peer-networks
- learning traffic controls
- robotic area scouts
- automation of processes in factories
- management of renewable energy resources
- self-repairing faulty systems in automobiles

Organic Computing

- goal: independent organization, configuration and repair of those complex IT systems
- solution: *Organic Computing*
  - adapt to (environmental) changes,
  - inspired by patterns in nature

problems:

- Controlling these systems becomes increasingly complex as they develop an emergent behaviour, i.e. a behaviour that they have not shown before
- emergence can be favorable, if the system is able to react correctly. Otherwise it might be fatal.
  Consider a learning traffic control system that switches all traffic lights to green because of noticing that letting cars pass is reducing traffic jams...

Organic Computing: More Than Just Optimization

- ants take on roles such as soldiers or workers
- e.g. if the number of soldiers drops below a certain threshold, some workers will become soldiers

$\Rightarrow$ sensors could take on new tasks when others fail

- systems could solve tasks easier and more efficiently after having performed on them several times before

- since 2004 the DFG supports fields regarding the topic Organic Computing
- literature: [Würtz, 2008] also online at `http://www.springerlink.com/content/978-3-540-77656-7`

Outline

Genetic and Evolutionary Algorithms

representation: (classical) $\{0,1\}^L$ with fixed length L (also $\mathbb{R}^L$ and $\mathcal{S}_n$, decoding)

mutation: bit flipping, uniformly distributed real-valued mutation, special operations for permutation

recombination: k-point- and uniform crossover, arithmetical crossover, order-based recombination

selection: parental selection, fitnessproportional or tournament selection

population: mid-sized populations

features: theoretical basis in Schema Theorem (*next up in the lecture*)

Local Search

representation: arbitrary

mutation: arbitrary

recombination: none

selection: improvements always, degradiation with a certain probability

population: one individual

features: early convergence is a central problem

Tabu Search

representation: close to phenotype

mutation: non-invertable because of Tabu-lists

recombination: none

selection: best individual

population: one parental, several children

features: best found individual is stored additionally

Memetic Algorithm

representation: arbitrary

mutation: combined with local search

recombination: arbitrary

selection: arbitrary

population: arbitrary

features: arbitrary

Differential evolution

representation: $\mathbb{R}^L$

mutation: mixed operator

recombination: mixed operator

selection: child replaces parental if it is superior

Population: small/mid-sized

features: mutation makes use of population information

Scatter Search

representation: $\mathbb{R}^L$ and others

mutation: none

recombination: subset operator and combination

selection: selection of the best

population: mid-sized

features: many variants, deterministic procedure

Cultural Algorithm

representation: $\mathbb{R}^L$ and others

mutation: makes use of conviction space

recombination: none

selection: environmental selection

population: mid-sized

features: conviction space stores prescriptive and situation-based information

Population-Based Incremental Learning

representation: $\{0, 1\}^L$

mutation: changing the population statistics

recombination: implicitly

selection: best child individual enters statistics

population: is replaced by population statistics

features: whenever individuals are needed, they are drawn from the statistics

Ant colony optimization

representation: several different

mutation: every ant generates one solution candidate

recombination: none

selection: quality determines influence on global pheromones

population: quantity of ants during one iteration

features: global amount of pheromones represents candidate solutions similar to statistics in PBIL

Particle Swarm Optimization

representation: $\mathbb{R}^L$

mutation: based on lethargy and neighbors

recombination: none

selection: based on the best (population/own memory)

population: small/mid-sized

features: synchronously searching the search space

literature for this lecture

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