



*Parallel Cooperative
Optimization Research
Group*

Metaheuristics for Optimization

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INRIA

Introduction (1)

- High-dimensional and complex optimization problems in many areas of industrial concern
→ Telecommunication, Computational biology, Transportation and Logistics, Design, ...
- Problems of increasing size (combinatorial explosion)
 - Getting near-optimal solutions in a tractable time
- Using approached methods isn't sufficient
 - Metaheuristics approach
 - Hybridization features
 - Large scale parallelism (Cluster & GRID Computing)

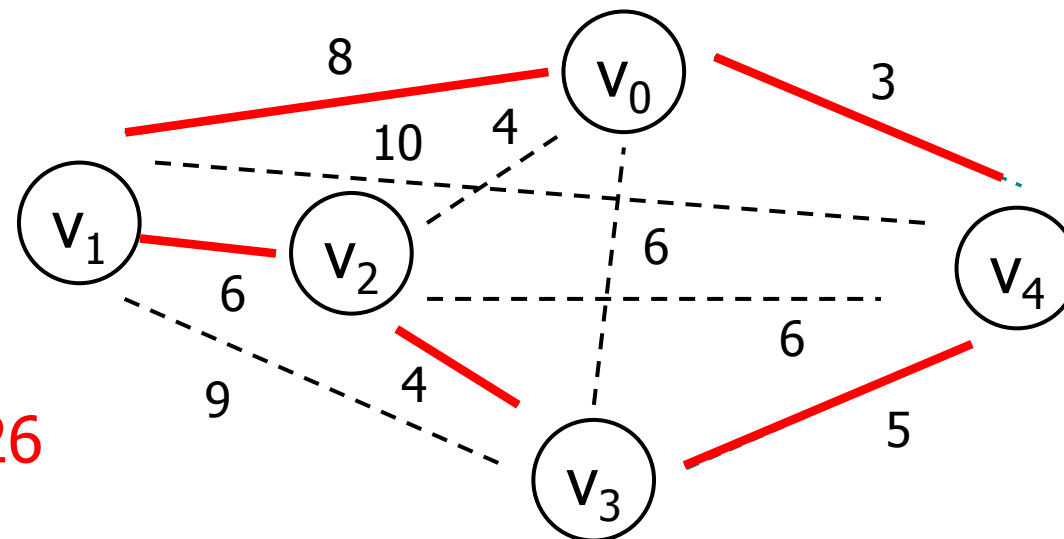
Popular NP-hard problems

- Permutation problems : traveling salesman, scheduling, ...
- Assignment : QAP, GAP, ...
- Grouping : partitioning, clustering, graph coloring ...
- Routing : VRP, CTP, ...
- Knapsack and packing

- and many more, etc

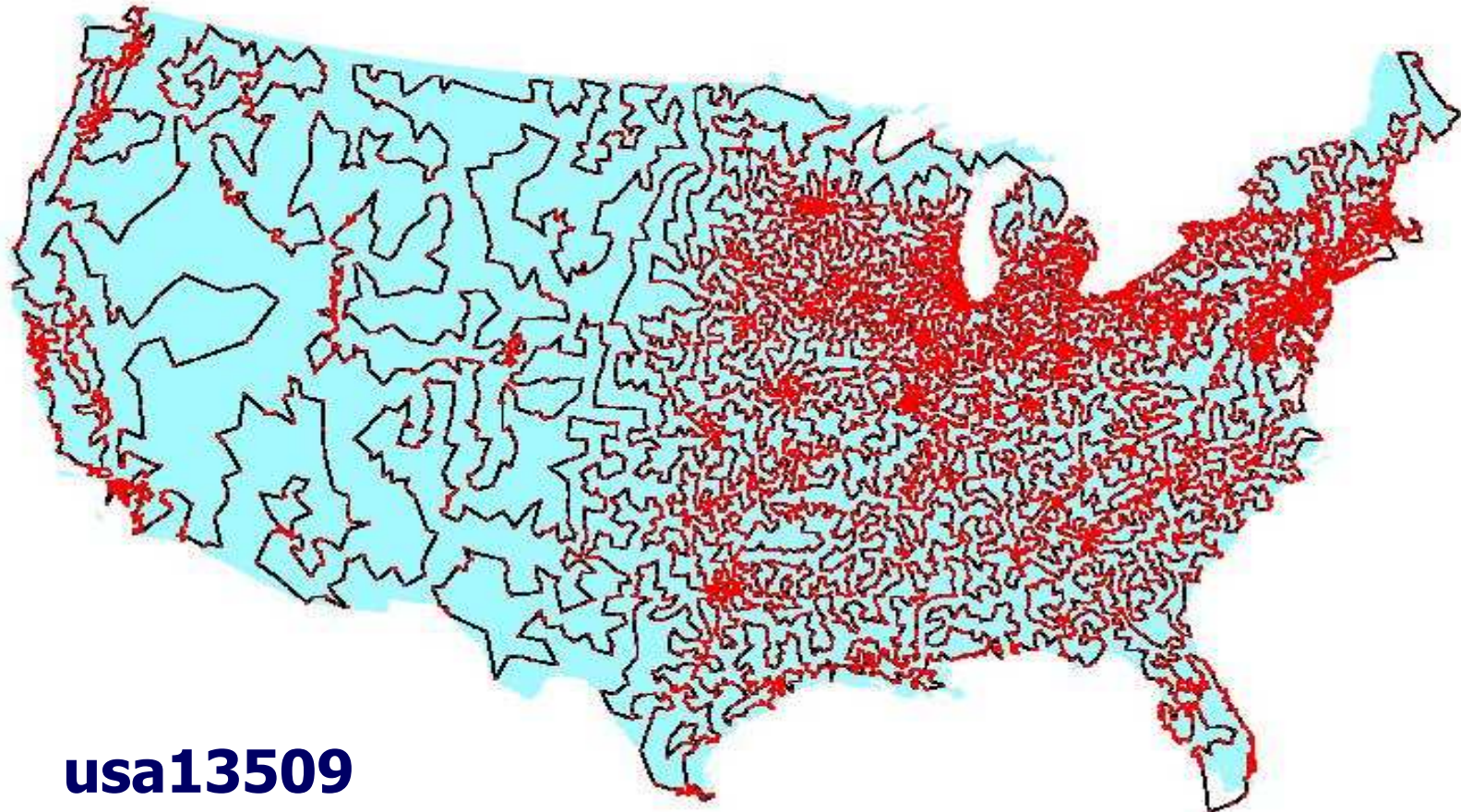
Tackling an academic COP. The Traveling Salesman Problem

- “Given a collection of N cities and the distance between each pair of them, the **TSP** aims at finding the shortest route visiting all of the cities”
- Symmetric TSP: $\frac{(N-1)!}{2}$ candidate solutions
- Example



Length: 26

Tackling an academic COP. The Traveling Salesman Problem



Tackling a real-world COP. Design of cellular radio networks

- Financial context (cost of the network)
 - Number of sites
 - Quality of Service
- Network design
 - Positioning sites
 - Fixing a set of parameters for each antenna
- Very highly combinatorial (NP-hard)



A practical hard problem

- Three main features
 - A high number of potential configurations
→ $\cong 4.8 \times 10^{2558}$, 8.4×10^{6494} and 5.5×10^{8541}
candidate solutions (on different instances
Arno 1.0, 3.0 et 3.1)
 - A CPU cost evaluation function (trigonometric
functions, sorting algorithms, ...).
 - Need of a large amount of memory
→ 512 Mo., 1 Go. and 2 Go.

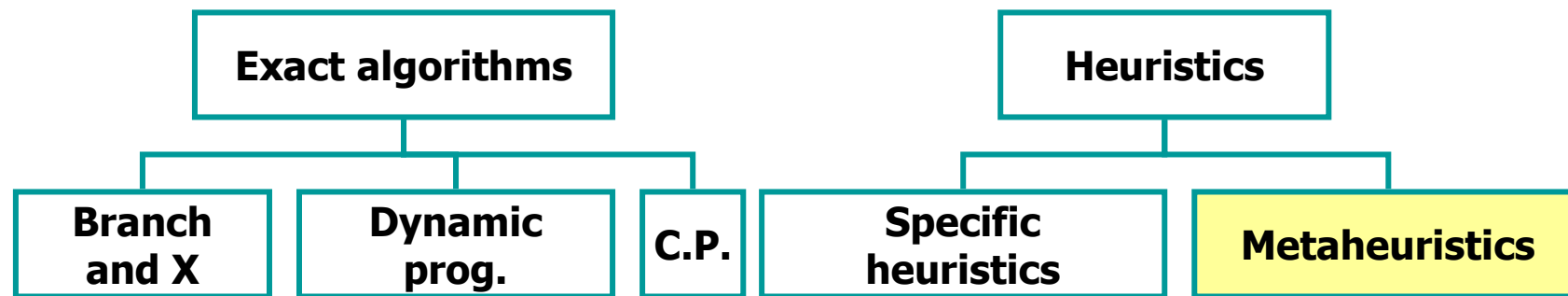
Introduction (2)

- Combinatorial Optimization Problems (COPs) in practice
 - Diversity
 - Continual **evolution** of the **modeling** (regards needs, objectives, constraints, ...)
 - **Need to experiment** many solving methods, techniques of hybridization, parameters, ...

Motivations

- A framework for the design of parallel hybrid metaheuristics dedicated to the mono/multi-objective resolution of COPs
 - Identifying abstract/specific features of both metaheuristics and main models of parallelization and hybridization
 - Insuring transparency of parallelism
 - Easily deploying on sequential architectures, parallel/distributed platforms and meta-computing grids
 - Validating the framework by tackling hard and real applications (modeling and solving)

Taxonomy (optimization methods)

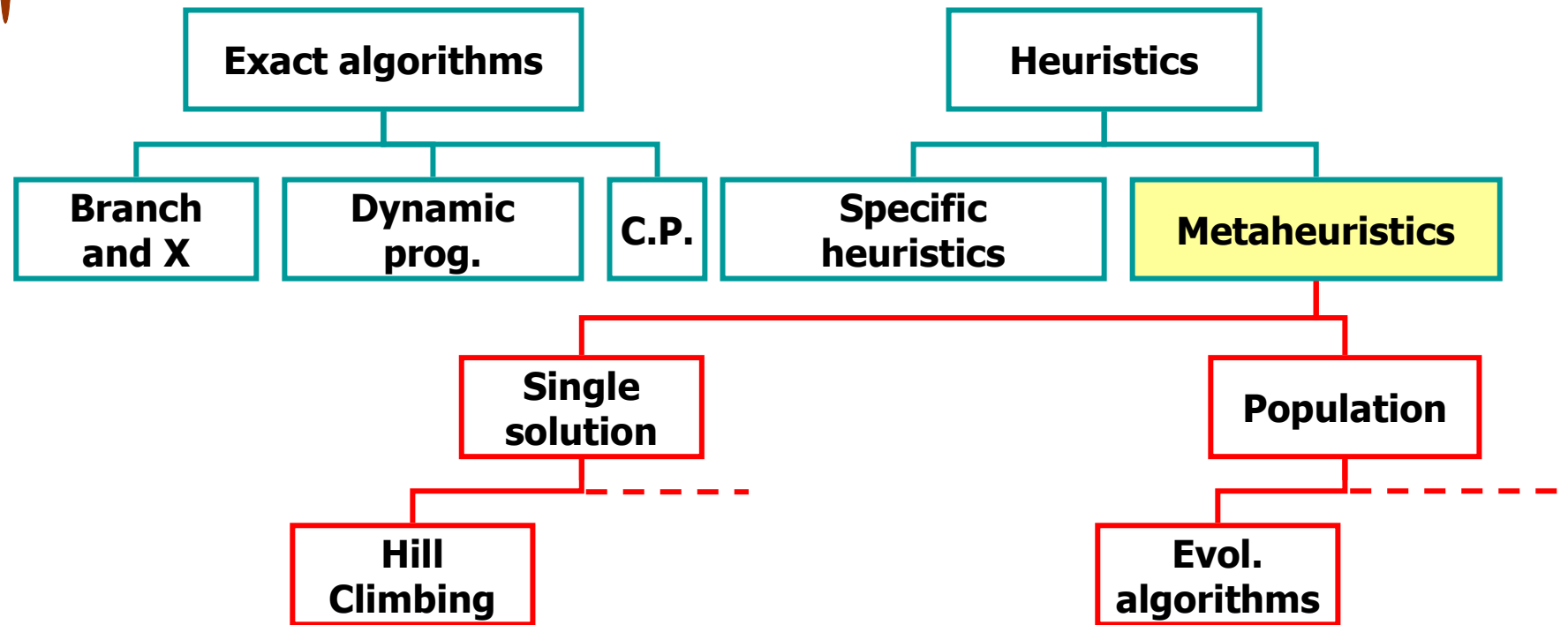


- Exact methods: optimality and exploitation on small instances
- Heuristics: near-optimal solutions on large-size problem instances

Classification of metaheuristics

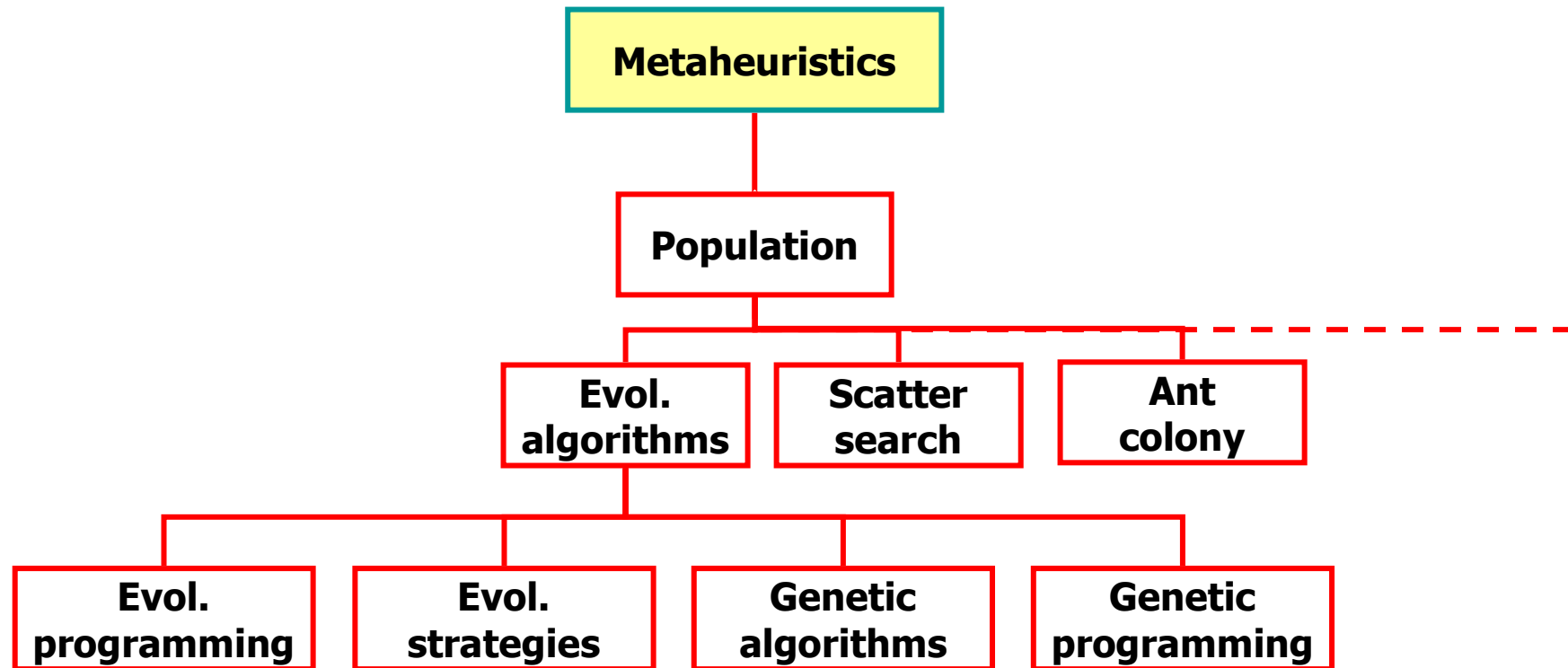
- Nature inspired vs. non nature inspired
- Population-based vs. single point search
- Dynamic vs. static objective function
- One vs. various neighborhood structures
- Memory usage vs. memory less methods
- Iterative vs. Greedy
- ...

Taxonomy (metaheuristics)



- Single solution metaheuristics are **exploitation** oriented
- Population-based metaheuristics are **exploration** oriented

Taxonomy (Population-based Metaheuristics)



Evolutionary Computation

History

- L. Fogel 1962 (San Diego, CA):
Evolutionary Programming
- J. Holland 1962 (Ann Arbor, MI):
Genetic Algorithms
- I. Rechenberg & H.-P. Schwefel 1965
(Berlin, Germany): *Evolution Strategies*
- J. Koza 1989 (Palo Alto, CA):
Genetic Programming

The metaphor

Evolution

Individual

Fitness

Environment



Problem solving

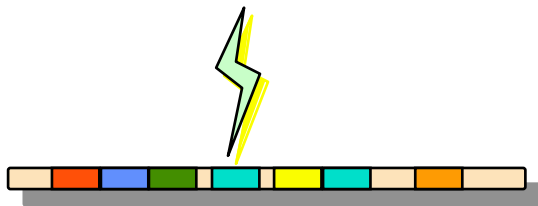
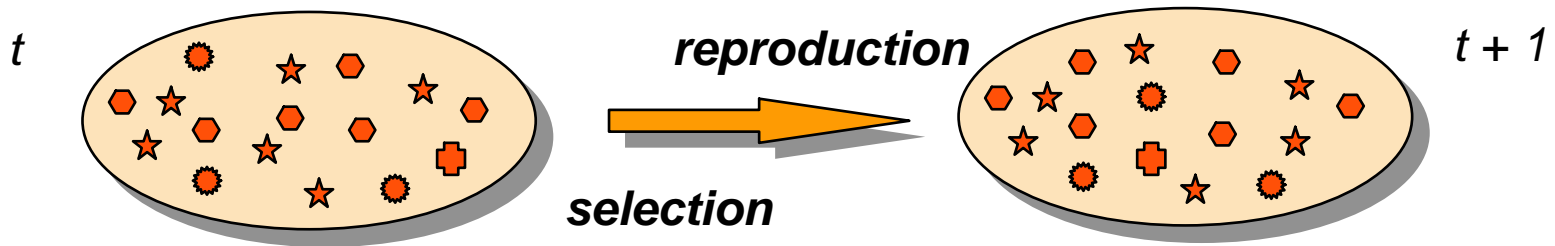
Candidate Solution

Quality

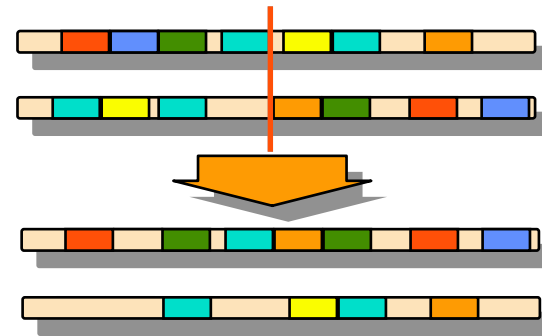
Problem

- Based on the evolution of a population of individuals
- Evolution features
 - Variation operators (crossover, mutation) to increase diversity,
 - Selection of parents, replacement by offspring to decrease diversity

The ingredients

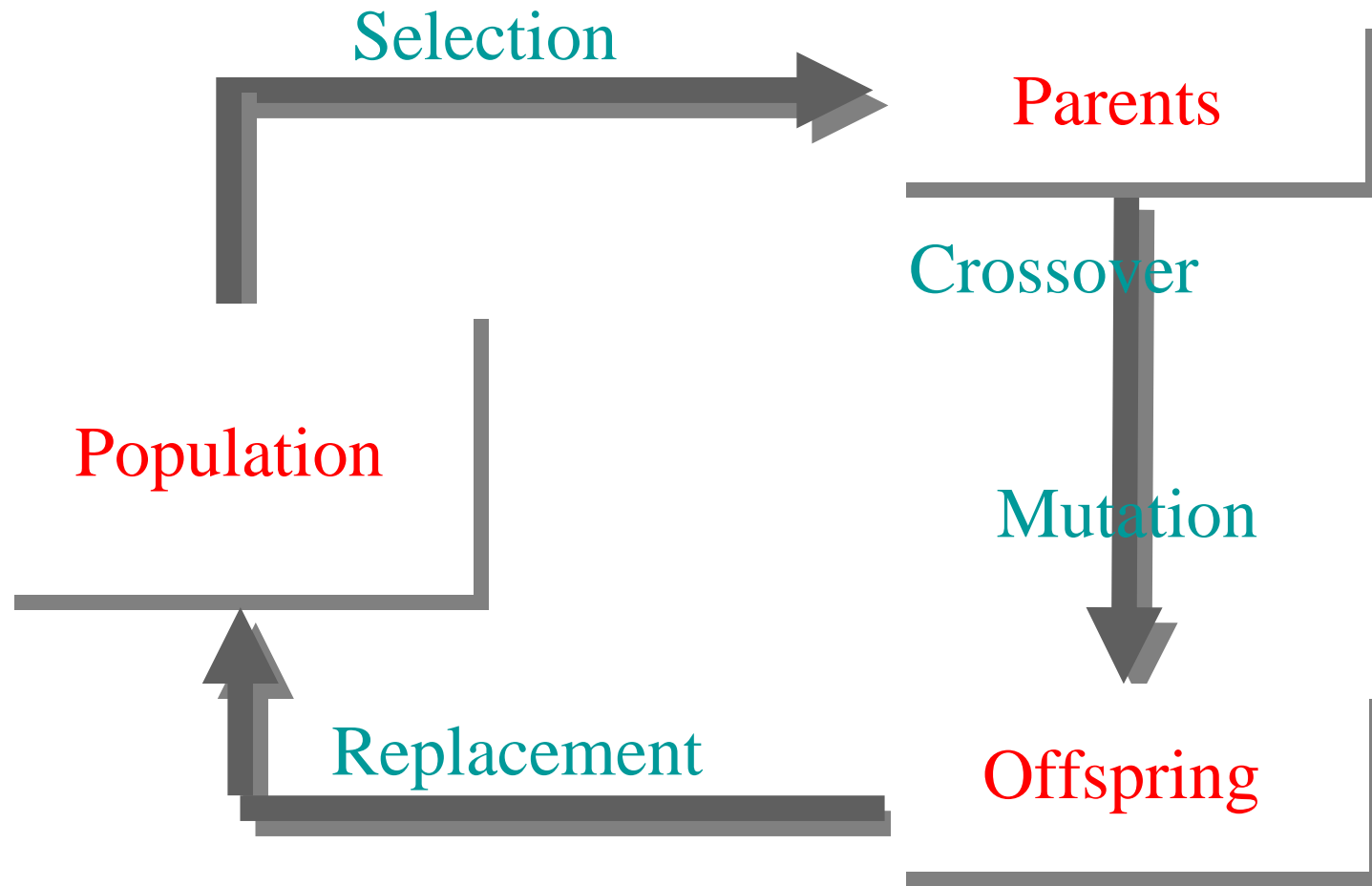


mutation



recombination

Evolutionary cycle



Evolutionary Algorithm procedure

- $t \leftarrow 0$
- $P \leftarrow \text{GenerateInitialPopulation} ()$
- evaluate (P_t)
- do
 - Select P_{t+1} from P_t
 - Transform (P_t)
 - Evaluate (P_t)
 - $P_{t+1} \leftarrow \text{Replace} (P_t, P_{t+1})$
 - $t \leftarrow t + 1$
- While termination conditions not met

Domains of application

- Numerical, Combinatorial Optimisation
- System Modeling and Identification
- Planning and Control
- Engineering Design
- Data Mining
- Machine Learning
- Artificial Life
- ...

Performances

- Acceptable performance at acceptable costs on a wide range of problems
- Intrinsic parallelism (robustness, fault tolerance)
- Superior to other techniques on complex problems with
 - lots of data, many free parameters
 - complex relationships between parameters
 - many (local) optima

Advantages

- No presumptions w.r.t. problem space
- Widely applicable
- Low development & application costs
- Easy to incorporate other methods
- Solutions are interpretable (unlike NN)
- Can be run interactively, accommodate user proposed solutions
- Provide many alternative solutions
- Robust regards any change of the environment (data, objectives, etc)
- Co-evolution, parallelism and distribution ...

Disadvantages

- No guarantee for optimal solution within finite time (in general)
- May need parameter tuning
- Often computationally expensive, i.e. slow

Genetic Algorithms

- Developed: USA in the 1970's
- Early names: J. Holland, K. DeJong, D. Goldberg
- Typically applied to:
 - discrete optimization
- Attributed features:
 - not too fast
 - good heuristic for combinatorial problems
- Special Features:
 - Traditionally emphasizes combining information from good parents (crossover)
 - many variants, e.g., reproduction models, operators

Genetic Algorithms (SGA)

Representation	Binary strings
Recombination	N-point or uniform
Mutation	Bitwise bit-flipping with fixed probability
Parent selection	Fitness-Proportionate
Survivor selection	All children replace parents
Speciality	Emphasis on crossover

Evolution Strategies

- Developed: Germany in the 1970's
- Early names: I. Rechenberg, H.-P. Schwefel
- Typically applied to:
 - numerical optimisation
- Attributed features:
 - fast
 - good optimizer for real-valued optimisation
 - relatively much theory
- Special:
 - self-adaptation of (mutation) parameters standard

Evolution Strategies

Representation	Real-valued vectors
Recombination	Discrete or intermediary
Mutation	Gaussian perturbation
Parent selection	Uniform random
Survivor selection	(μ, λ) or $(\mu + \lambda)$
Specialty	Self-adaptation of mutation step sizes

Evolutionary Programming

- Developed: USA in the 1960's
- Early names: D. Fogel
- Typically applied to:
 - traditional EP: machine learning tasks by finite state machines
 - contemporary EP: (numerical) optimization
- Attributed features:
 - very open framework: any representation and mutation op's OK
 - crossbred with ES (contemporary EP)
 - consequently: hard to say what "standard" EP is
- Special:
 - no recombination
 - self-adaptation of parameters standard (contemporary EP)

Evolutionary Programming

Representation	Real-valued vectors
Recombination	None
Mutation	Gaussian perturbation
Parent selection	Deterministic
Survivor selection	Probabilistic ($\mu+\mu$)
Specialty	Self-adaptation of mutation step sizes (in meta-EP)

Genetic Programming

- Developed: USA in the 1990's
- Early names: J. Koza
- Typically applied to:
 - machine learning tasks (prediction, classification...)
- Attributed features:
 - competes with neural nets and alike
 - needs huge populations (thousands)
 - slow
- Special:
 - non-linear chromosomes: trees, graphs
 - mutation possible but not necessary (disputed!)

Genetic Programming

Representation	Tree structures
Recombination	Exchange of subtrees
Mutation	Random change in trees
Parent selection	Fitness proportional
Survivor selection	Generational replacement

Books

- Th. Bäck, "Evolutionary Algorithms in Theory and Practice", *Oxford University Press, 1996*
- L. Davis, "The Handbook of Genetic Algorithms", *Van Nostrand & Reinhold, 1991*
- D.B. Fogel, "Evolutionary Computation", *IEEE Press, 1995*
- D.E. Goldberg, "Genetic Algorithms in Search, Optimisation and Machine Learning", *Addison-Wesley, 1989*
- J. Koza, "Genetic Programming", *MIT Press, 1992*
- Z. Michalewicz, "Genetic Algorithms + Data Structures = Evolution Programs", *Springer, 3rd ed., 1996*
- H.-P. Schwefel, "Evolution and Optimum Seeking", *Wiley & Sons, 1995*

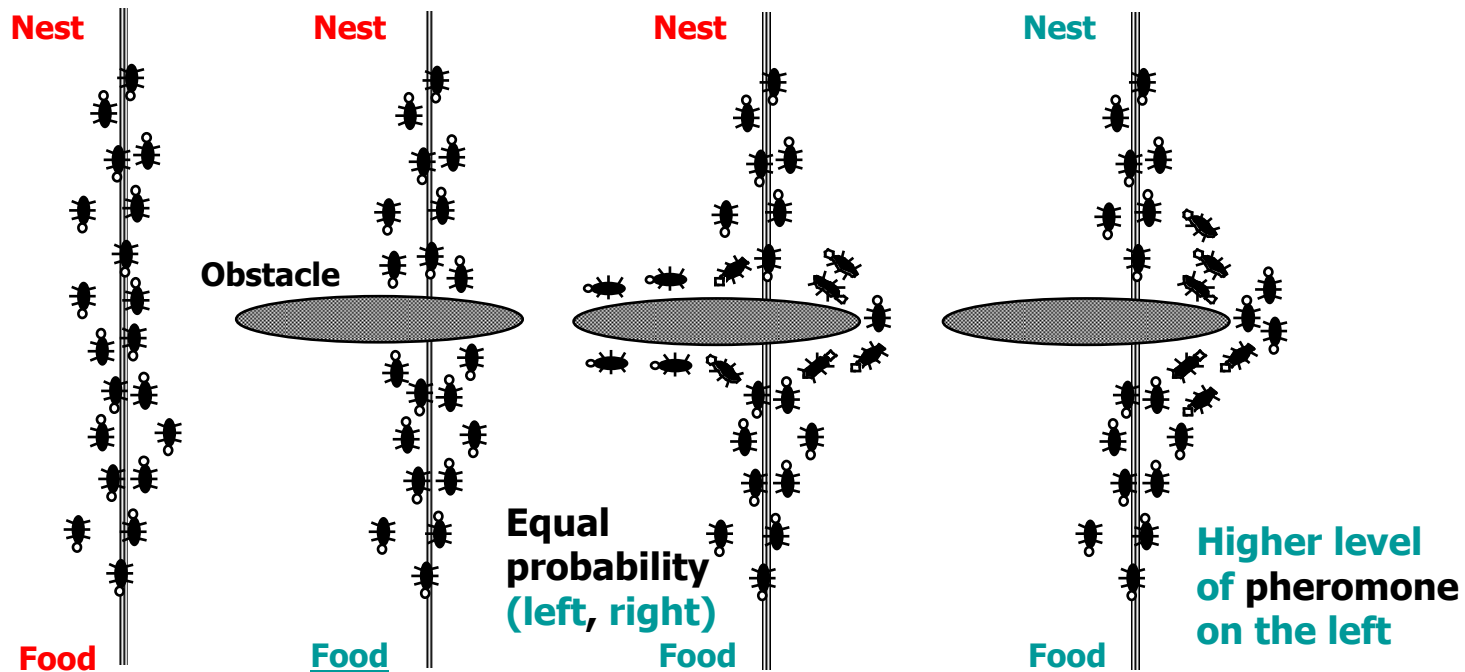
Ant colony Optimization (ACO)

Ant colonies

- Artificial ants: Dorigo (1992)
- Imitate the cooperative behavior of ant colonies to solve optimization problems
- Use very simple communication mechanism : pheromone
 - Olfactive and volatile substance
 - Evolution : evaporation, reinforcement

M. Dorigo, & G. Di Caro. "The Ant Colony Optimization Meta-heuristic".
New Ideas in Optimization, 1999

A nature-inspired process



- During the trip, a pheromone is left on the ground.
- The quantity left depends on the amount of food found.
- The path is chosen accordingly to the quantity of pheromones.
- The pheromone has a decreasing action over time.

Ant colony procedure

- Do
 - Schedule activities
 - AntBasedSolution Construction
 - Pheromone Update
 - Daemons Actions
- While termination conditions not met

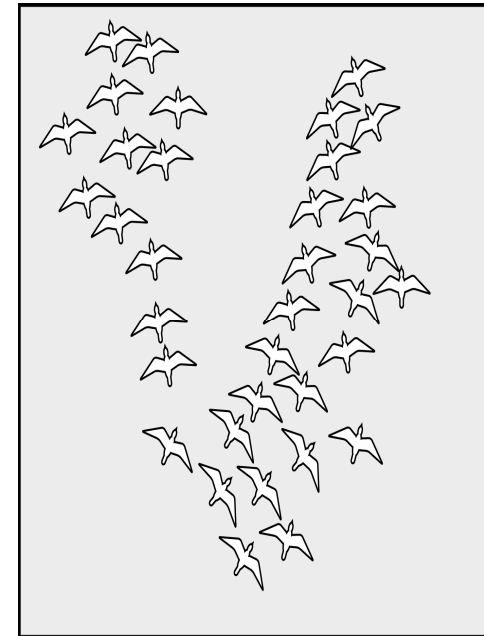
Application to Combinatorial Optimization Problems

- **Traveling Salesman Problem:** T. Stützle, 1997
- **Vehicle Routing Problem:** Hartl et al., 1997
- **Graph Coloring:** Costa et Hertz, 1997
- **Frequency Assignment Problem:** Dicaro et al., 1997
- **Quadratic Assignment Problem:**
Gambardella, Taillard et Dorigo, 1997
- **Set Covering:** E-G. Talbi et al., 1997
- **Graph Partitioning:** Kuntz et Snyers, 1994

Particle Swarm Optimization (PSO)

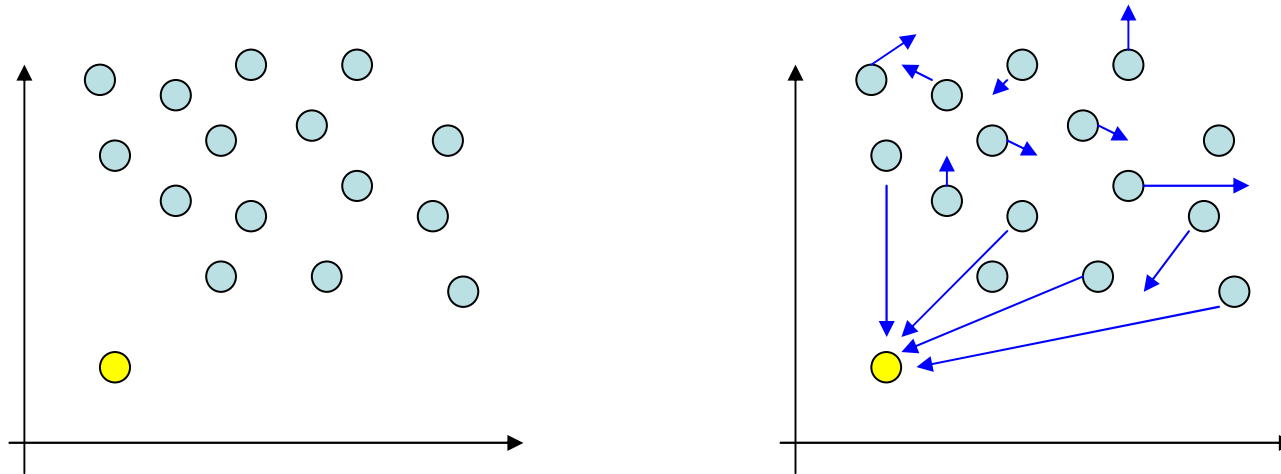
Particle Swarm

- Population based stochastic metaheuristic
- Dr. Eberhart and Dr. Kennedy (1995)
- Inspired by social behavior of bird flocking or fish schooling
- Similarities with genetic algorithm



Kennedy, J. and Eberhart, R. C., "The particle swarm: social adaptation in information processing systems," in Corne, D., Dorigo, M., and Glover, F. (eds.) New Ideas in Optimization London, UK: McGraw-Hill, 1999

A nature-inspired process



- Particles fly through the problem space
- Flight = add a velocity to the current position
- Social adaptation of knowledge
- Particles follow the current optimum particles («follow the bird which is nearest to the food »)

PSO procedure

- Do
 - Evaluate the velocities
 - Flight
 - Update the bests
- While termination conditions not met

Swarm construction

- Initialize positions P :

$$P_i = \text{random}$$

- Initialize the first best position P_{best} of each particle :

$$P_{i \text{ best}} = P_i \quad (\text{standard strategy})$$

- Initialize the global best P_{gbest} particle:

$$P_{\text{gbest}} = \text{best}(P_i) \quad (\text{standard strategy})$$

Make the particles flying

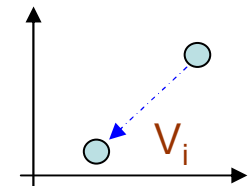
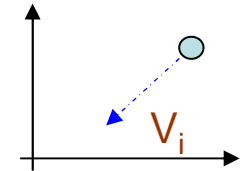
- Evaluate the velocities :

$$V_i = V_i + \underbrace{c_1 \times (P_{i\text{best}} - P_i)}_{\text{local direction}} + \underbrace{c_2 \times (P_{g\text{best}} - P_i)}_{\text{global direction}}$$

→ c_1 and c_2 = learning factors

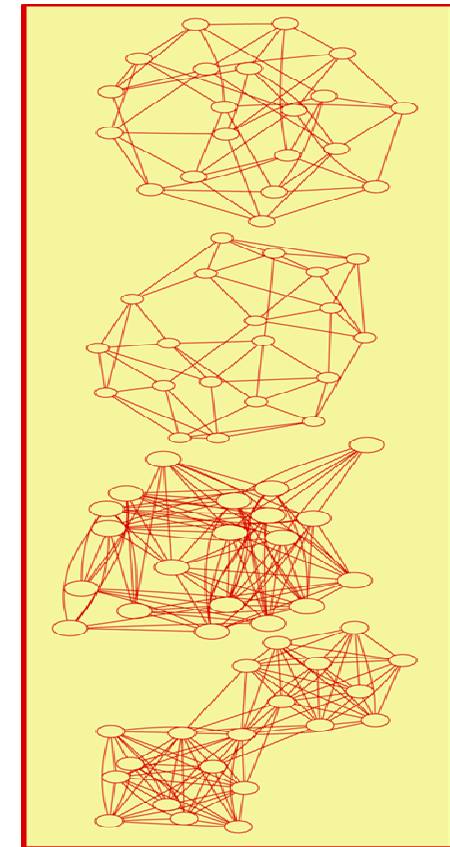
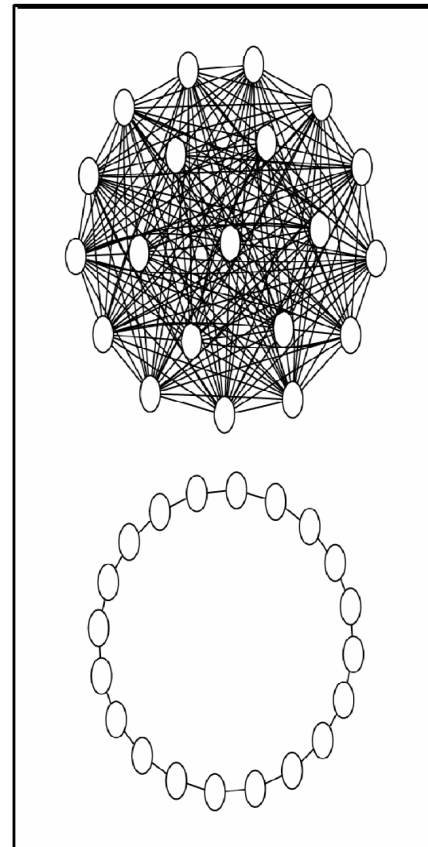
- Perform the flight

$$P_i = P_i + V_i$$



Topology

- Determines how the solution spread through the population
- Local, global, neighbourhood best ?
- Affects the rate of convergence
- Advanced parallel search



Mean degree, Clustering, Heterogeneity

Update the particle's best

- Update the best fitness value of each particle :

- *If P_i better than $P_{i\ best}$*
 $P_{i\ best} = P_i$

- Update the global best :

- *If P_i better than $P_{g\ best}$*
 $P_{g\ best} = P_i$

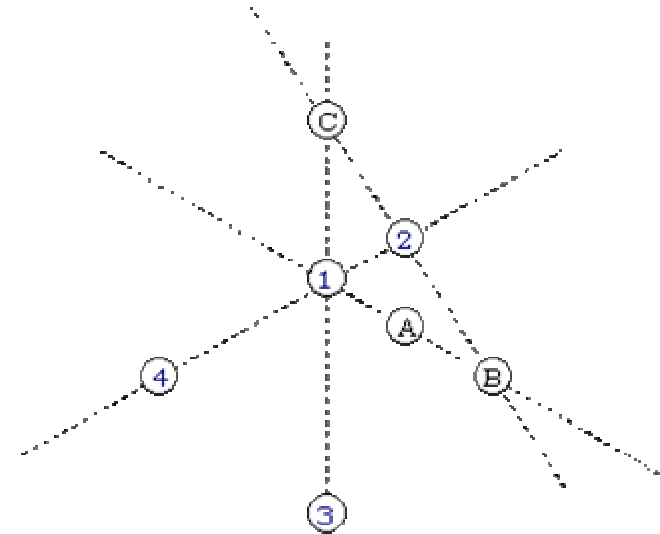
Application to Combinatorial Optimization Problems

- Transport : Venter, 2004
- Traveling salesman problem : Sofge, Schultz, 2003
- Planning : Onwubolu, G. C. and Clerc, 2004

Scatter search and path relinking

Scatter Search and Path Relinking

- Scatter Search and its generalized form Path Relinking provide unifying principles for joining (or recombining) solutions based on generalized path constructions in Euclidean or neighborhood spaces



F. Glover. "Scatter Search and Path relinking".

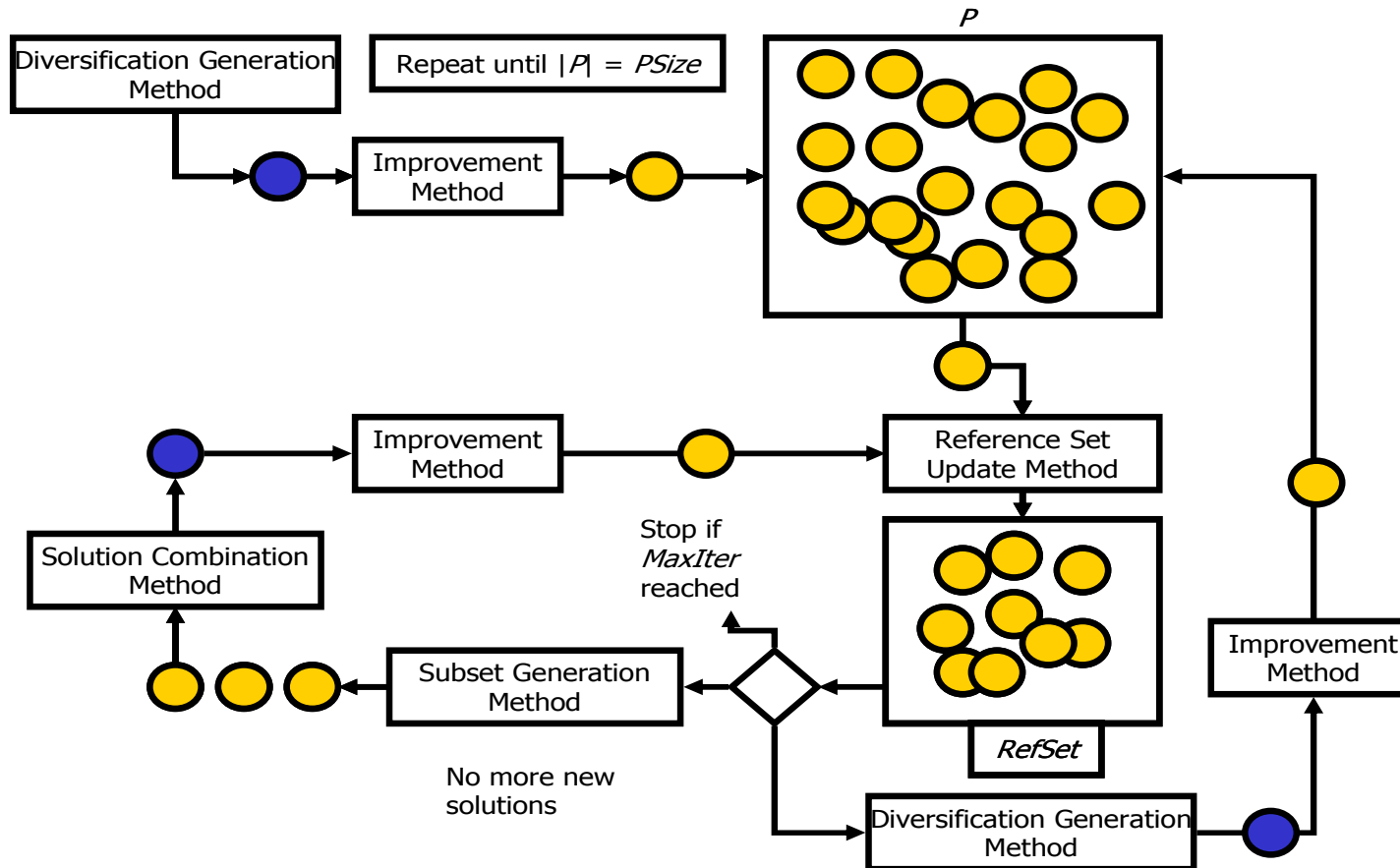
New ideas in optimization, Advanced topics in computer science series, 1999.

F. Glover, M. Laguna and R. Marti. "Fundamentals of scatter search and path relinking". Control and Cybernetic, 2000.

Main operators

- **Diversification Generation Method** : Generate a collection of diverse trial solutions
- **Improvement Method** : Transform a trial solution into one or more enhanced trial solutions
- **Reference Set Update Method** : Build and maintain a reference set - "best" solutions found (quality, diversity)
- **Subset Generation Method** : Operate on the reference set, to produce a subset of its solutions as a basis for creating combined solutions
- **Solution Combination Method** : Transform a given subset of solutions produced by the Subset Generation Method

Overview



Scatter Search procedure

- Create diversified population
- Generate Reference Set
- Do
 - Do
 - Subset Generation Method
 - Solution Combination Method
 - Improvement Method
 - Until first termination criterion is not reached
 - Reference Set Update Method
- Until other termination criterion is not reached

Estimation of Distribution Algorithm (EDA)

Estimation of Distribution Algorithm

- Based on the use of (unsupervised) density estimators/generative statistical models
- Idea is to convert the optimization problem into a search over probability distributions
- The probabilistic model is in some sense an explicit model of (currently) promising regions of the search space

EDA pseudo-code

- Initialize a probability model $Q(x)$
- Do
 - Create a population of points by sampling from $Q(x)$
 - Evaluate the objective function for each point
 - Update $Q(x)$ using selected population and $f()$ values
- While termination criterion not reached

EDA simplest probability model

- Population-based incremental Learning (PBIL)
 - Initial distribution $D=(0.5, \dots, 0.5)$
 - Boucle :
 - Generation of the population
 - $X_i = 1$ if $r < D_i$ (r uniform in $[0,1]$)
 - $X_i = 0$ else
 - Evaluate and sort the population
 - Update the distribution

$$D = (1 - \alpha)D + \alpha \cdot X_{best}$$

S. Baluja, R. Caruana. Removing the Genetics from the Standard Genetic Algorithm. ICML'95

Other probability models

- Mutual Information Maximization for Input Clustering (MIMIC) regards pairwise dependances

J. De Bonet, C. Isbell and P. Viola. MIMIC: Finding optima by estimating probability densities.

Advances in Neural Information Processing Systems, vol.9, 1997

- Bayesian Optimization Algorithm (BOA) for multivariate dependances

M. Pelikan, D. Goldberg and E. Cantu-Paz. BOA: The Bayesian optimization algorithm. In Proc. GECCO'99

EDA : Applications

- Field of EDA is quite young. Much effort is focused on methodology rather than performance
- First applications
 - Knapsack problem
 - Job Shop Scheduling