

## Variable Neighbourhood Search (VNS)

**Key Idea:** systematically change neighbourhoods during search

### Motivation:

- ▶ *recall*: changing neighbourhoods can help escape local optima
- ▶ a global optimum is locally optimal w.r.t. *all* neighbourhood structures
- ▶ *principle of VNS*: change the neighbourhood during the search

- ▶ main VNS variants
  - ▶ variable neighbourhood descent (VND, already discussed)
  - ▶ basic variable neighborhood search
  - ▶ reduced variable neighborhood search
  - ▶ variable neighborhood decomposition search

## How to generate the various neighborhood structures?

- ▶ for many problems different neighborhood structures (local searches) exist / are in use
- ▶ use  $k$ -exchange neighborhoods; these can be naturally extended
- ▶ many neighborhood structures are associated with distance measures: define neighbourhoods in dependence of the distances between solutions

## basic VNS

- ▶ uses neighborhood structures  $\mathcal{N}_k, k = 1, \dots, k_{max}$
- ▶ iterative improvement in  $\mathcal{N}_1$
- ▶ other neighborhoods are explored only randomly
- ▶ exploration in other neighborhoods are perturbations in the ILS sense
- ▶ perturbation is systematically varied
- ▶ acceptance criterion  $\text{Better}(s^*, s^{*'})$

## Basic VNS — Procedural view

### procedure *basic VNS*

```
 $s_0 \leftarrow \text{GenerateInitialSolution, choose } \{\mathcal{N}_k\}, k = 1, \dots, k_{\max}$   
repeat  
   $s' \leftarrow \text{RandomSolution}(\mathcal{N}_k(s^*))$   
   $s^{*'} \leftarrow \text{LocalSearch}(s')$  % local search w.r.t.  $\mathcal{N}_1$   
  if  $f(s^{*'}) < f(s^*)$  then  
     $s^* \leftarrow s^{*'}$   
     $k \leftarrow 1$   
  else  
     $k \leftarrow k + 1$   
until termination condition  
end
```

## Basic VNS — variants

- ▶ order of the neighborhoods
  - ▶ forward VNS: start with  $k = 1$  and increase  $k$  by one if no better solution is found; otherwise set  $k \leftarrow 1$
  - ▶ backward VNS: start with  $k = k_{\max}$  and decrease  $k$  by one if no better solution is found
  - ▶ extended version: parameters  $k_{\min}$  and  $k_{\text{step}}$ ; set  $k \leftarrow k_{\min}$  and increase  $k$  by  $k_{\text{step}}$  if no better solution is found
- ▶ acceptance of worse solutions
  - ▶ Skewed VNS: accept if

$$f(s^{*'}) - \alpha d(s^*, s^{*'}) < f(s^*)$$

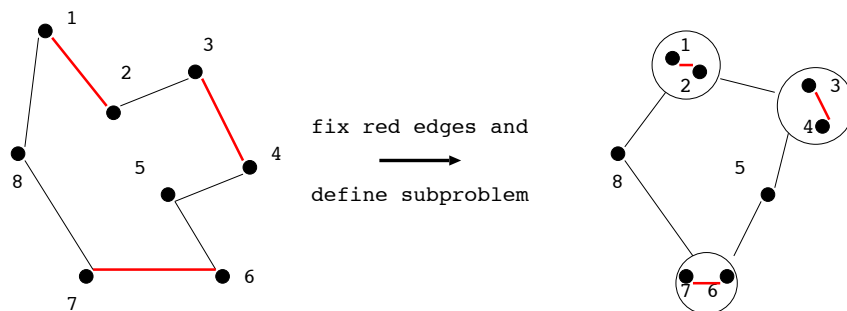
$d(s^*, s^{*'})$  measures distance between candidate solutions

## Reduced VNS

- ▶ same as basic VNS except that no iterative improvement procedure is applied
- ▶ only explores randomly different neighborhoods
- ▶ goal: reach quickly good quality solutions for large instances

## Variable Neighborhood Decomposition Search

- ▶ *central idea*
  - ▶ generate subproblems by keeping all but  $k$  solution components fixed
  - ▶ apply local search only to the  $k$  “free” components



- ▶ related approaches: POPMUSIC, MIMAUSA, etc.

## VNDS — Procedural view

**procedure** *VNDS*

$s_0 \leftarrow \text{GenerateInitialSolution}$ , choose  $\{\mathcal{N}_k\}$ ,  $k = 1, \dots, k_{\max}$

**repeat**

$s' \leftarrow \text{RandomSolution}(\mathcal{N}_k(s))$

$t \leftarrow \text{DetermineFreeComponents}(s', s)$

$t^* \leftarrow \text{LocalSearch}(t)$  % local search w.r.t.  $\mathcal{N}_k$

$s'' \leftarrow \text{InjectComponents}(t^*, s')$

**if**  $f(s'') < f(s)$  **then**

$s \leftarrow s''$

$k \leftarrow 1$

**else**

$k \leftarrow k + 1$

**until** *termination condition*

**end**

## relationship between ILS and VNS

- ▶ the two SLS methods are based on different underlying “philosophies”
- ▶ they are similar in many respects
- ▶ ILS appears to be in literature more flexible w.r.t. optimization of the interaction of modules
- ▶ VNS gives place to approaches like VND for obtaining more powerful local search approaches

## Greedy Randomised Adaptive Search Procedures

**Key Idea:** Combine randomised constructive search with subsequent perturbative local search.

### Motivation:

- ▶ Candidate solutions obtained from construction heuristics can often be substantially improved by perturbative local search.
- ▶ Perturbative local search methods typically often require substantially fewer steps to reach high-quality solutions when initialised using greedy constructive search rather than random picking.
- ▶ By iterating cycles of constructive + perturbative search, further performance improvements can be achieved.

### Greedy Randomised “Adaptive” Search Procedure (GRASP):

While *termination criterion* is not satisfied:

- generate candidate solution  $s$  using  
*subsidiary greedy randomised constructive search*
- perform *subsidiary local search* on  $s$

### Note:

Randomisation in *constructive search* ensures that a large number of good starting points for *subsidiary local search* is obtained.

## Restricted candidate lists (RCLs)

- ▶ Each step of *constructive search* adds a solution component selected uniformly at random from a *restricted candidate list (RCL)*.
- ▶ RCLs are constructed in each step using a *heuristic function*  $h$ .
- ▶ RCLs based on *cardinality restriction* comprise the  $k$  best-ranked solution components. ( $k$  is a parameter of the algorithm.)
- ▶ RCLs based on *value restriction* comprise all solution components  $l$  for which  $h(l) \leq h_{min} + \alpha \cdot (h_{max} - h_{min})$ , where  $h_{min}$  = minimal value of  $h$  and  $h_{max}$  = maximal value of  $h$  for any  $l$ . ( $\alpha$  is a parameter of the algorithm.)

### Note:

- ▶ Constructive search in GRASP is 'adaptive':  
Heuristic value of solution component to be added to given partial candidate solution  $r$  may depend on solution components present in  $r$ .
- ▶ Variants of GRASP without perturbative local search phase (aka *semi-greedy heuristics*) typically do not reach the performance of GRASP with perturbative local search.

## Example: GRASP for SAT [Resende and Feo, 1996]

- ▶ **Given:** CNF formula  $F$  over variables  $x_1, \dots, x_n$
- ▶ **Subsidiary constructive search:**
  - ▶ start from empty variable assignment
  - ▶ in each step, add one atomic assignment (*i.e.*, assignment of a truth value to a currently unassigned variable)
  - ▶ heuristic function  $h(i, v) :=$  number of clauses that become satisfied as a consequence of assigning  $x_i := v$
  - ▶ RCLs based on cardinality restriction (contain fixed number  $k$  of atomic assignments with largest heuristic values)
- ▶ **Subsidiary local search:**
  - ▶ iterative best improvement using 1-flip neighbourhood
  - ▶ terminates when model has been found or given number of steps has been exceeded

GRASP has been applied to many combinatorial problems, including:

- ▶ SAT, MAX-SAT
- ▶ the Quadratic Assignment Problem
- ▶ various scheduling problems

## Extensions and improvements of GRASP:

- ▶ reactive GRASP (*e.g.*, dynamic adaptation of  $\alpha$  during search)
- ▶ combinations of GRASP with tabu search, path relinking and other SLS methods



## Iterated Greedy

**Key Idea:** iterate over greedy construction heuristics through destruction and construction phases

### Motivation:

- ▶ start solution construction from partial solutions to avoid reconstruction from scratch
  - ▶ keep features of the best solutions to improve solution quality
  - ▶ if few construction steps are to be executed, greedy heuristics are fast
- ▶ adding a subsidiary local search phase may further improve performance

### Iterated Greedy (IG):

While *termination criterion* is not satisfied:

    | generate candidate solution  $s$  using  
    | *subsidiary greedy constructive search*

While termination criterion is not satisfied:

    |  $r := s$   
    | apply *solution destruction* on  $s$   
    | perform *subsidiary greedy constructive search* on  $s$   
  
    | based on *acceptance criterion*,  
    | keep  $s$  or revert to  $s := r$

### Note:

- ▶ subsidiary local search after solution reconstruction can substantially improve performance

## Iterated Greedy (IG):

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        keep  $s$  or revert to  $s := r$

### Note:

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## IG—main issues

- ▶ destruction phase
  - ▶ fixed vs. variable size of destruction
  - ▶ stochastic vs. deterministic destruction
  - ▶ uniform vs. biased destruction
- ▶ construction phase
  - ▶ not every construction heuristic is necessarily useful
  - ▶ typically, adaptive construction heuristics preferable
  - ▶ speed of the construction heuristic is an issue
- ▶ acceptance criterion
  - ▶ very much the same issue as in ILS

## IG — enhancements

- ▶ usage of history information to bias destructive/constructive phase
- ▶ combination with local search in the constructive phase
- ▶ use local search to improve full solutions  
     $\rightsquigarrow$  destruction / construction phases can be seen as a perturbation mechanism in ILS
- ▶ usage of elements of tree search algorithms such as lower bounds on the completion of a solution or constraint propagation techniques

## Example: IG for SCP [Jacobs, Brusco, 1995]

- ▶ **Given:**
  - ▶ finite set  $\mathbf{A} = \{a_1, \dots, a_m\}$  of objects
  - ▶ family  $\mathbf{B} = \{B_1, \dots, B_n\}$  of subsets of  $\mathbf{A}$  that covers  $\mathbf{A}$
  - ▶ weight function  $w : \mathbf{B} \mapsto \mathbb{R}^+$
- ▶  $\mathbf{C} \subseteq \mathbf{B}$  covers  $\mathbf{A}$  if every element in  $\mathbf{A}$  appears in at least one set in  $\mathbf{C}$ , i.e. if  $\bigcup \mathbf{C} = \mathbf{A}$
- ▶ **Goal:**
  - ▶ find a subset  $\mathbf{C}^* \subseteq \mathbf{B}$  of minimum total weight that covers  $\mathbf{A}$ .

## Example: IG for SCP, continued ..

- ▶ assumption: all subsets from **B** are ordered according to nondecreasing costs
- ▶ construct initial solution using a greedy heuristic based on two steps
  - ▶ randomly select an uncovered object  $a_i$
  - ▶ add the lowest cost subset that covers  $a_i$
- ▶ the *destruction phase* removes a fixed number of  $k_1|\mathbf{C}|$  subsets;  $k_1$  is a parameter

- ▶ the *construction phase* proceeds as
  - ▶ build a candidate set containing subsets with cost of less than  $k_2 \cdot f(\mathbf{C})$
  - ▶ compute cover value  $\gamma_j = w_j/d_j$   
 $d_j$ : number of additional objects covered by adding subset  $b_j$
  - ▶ add a subset with minimum cover value
- ▶ complete solution is post-processed by removing redundant subsets
- ▶ *acceptance criterion*: Metropolis condition from PII
- ▶ computational experience
  - ▶ good performance with this simple approach
  - ▶ more recent IG variants are state-of-the-art algorithms for SCP

- ▶ IG has been re-invented several times; names include
  - ▶ simulated annealing, ruin-and-recreate, iterative flattening, iterative construction search, large neighborhood search, ..
- ▶ close relationship to iterative improvement in large neighbourhoods
- ▶ analogous extension to greedy heuristics as ILS to local search
- ▶ for some applications so far excellent results
- ▶ can give lead to effective combinations of tree search and local search heuristics

## Population-based SLS Methods

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SLS methods discussed so far manipulate one candidate solution of given problem instance in each search step.

**Straightforward extension:** Use *population* (i.e., set) of candidate solutions instead.

### Note:

- ▶ The use of populations provides a generic way to achieve search diversification.
- ▶ Population-based SLS methods fit into the general definition from Chapter 1 by treating sets of candidate solutions as search positions.

## Ant Colony Optimisation (1)

**Key idea:** Can be seen as population-based constructive approach where a population of agents – (*artificial*) *ants* – communicate via common memory – (*simulated*) *pheromone trails*.

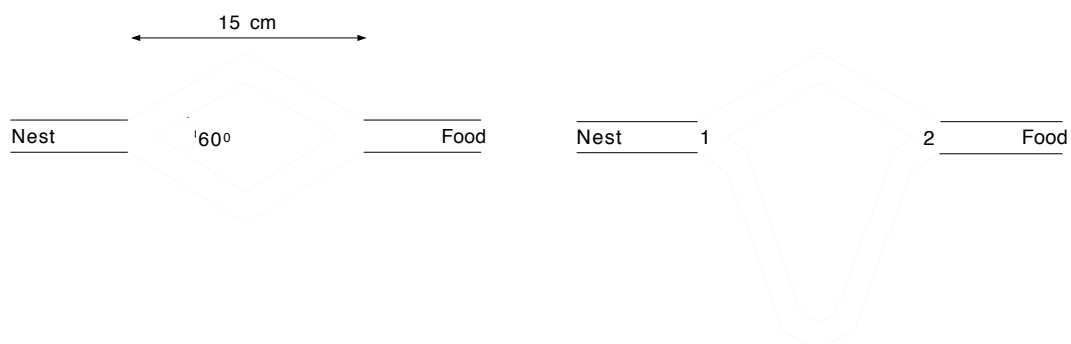
### Inspired by foraging behaviour of real ants:

- ▶ Ants often communicate via chemicals known as *pheromones*, which are deposited on the ground in the form of trails. (This is a form of *stigmergy*: indirect communication via manipulation of a common environment.)
- ▶ Pheromone trails provide the basis for (stochastic) trail-following behaviour underlying, e.g., the collective ability to find shortest paths between a food source and the nest.

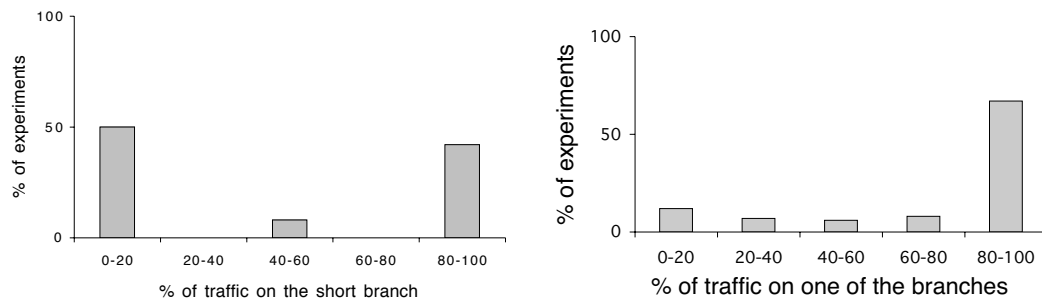
## Double bridge experiments Deneubourg++

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- ▶ laboratory colonies of *Iridomyrmex humilis*
- ▶ ants deposit pheromone while walking from food sources to nest *and* vice versa
- ▶ ants tend to choose, in probability, paths marked by strong pheromone concentrations



- ▶ equal length bridges: convergence to a single path
- ▶ different length paths: convergence to short path



- ▶ a stochastic model was derived from the experiments and verified in simulations
- ▶ functional form of transition probability

$$p_{i,a} = \frac{(k + \tau_{i,a})^\alpha}{(k + \tau_{i,a})^\alpha + (k + \tau_{i,a'})^\alpha}$$

- ▶  $p_{i,a}$ : probability of choosing branch  $a$  when being at decision point  $i$   
 $\tau_{i,a}$ : corresponding pheromone concentration
- ▶ good fit to experimental data with  $\alpha = 2$

## Towards artificial ants

- ▶ real ant colonies are solving *shortest path problems*
- ▶ ACO takes elements from real ant behavior to solve more complex problems than real ants
- ▶ In ACO, artificial ants are *stochastic solution construction procedures* that probabilistically build solutions exploiting
  - ▶ (artificial) *pheromone trails* that change at run time to reflect the agents' acquired search experience
  - ▶ *heuristic information* on the problem instance being solved

## Ant Colony Optimisation

### **Application to combinatorial problems:**

[Dorigo et al. 1991, 1996]

- ▶ Ants iteratively construct candidate solutions.
- ▶ Solution construction is probabilistically biased by pheromone trail information, heuristic information and partial candidate solution of each ant.
- ▶ Pheromone trails are modified during the search process to reflect collective experience.



## Ant Colony Optimisation (ACO):

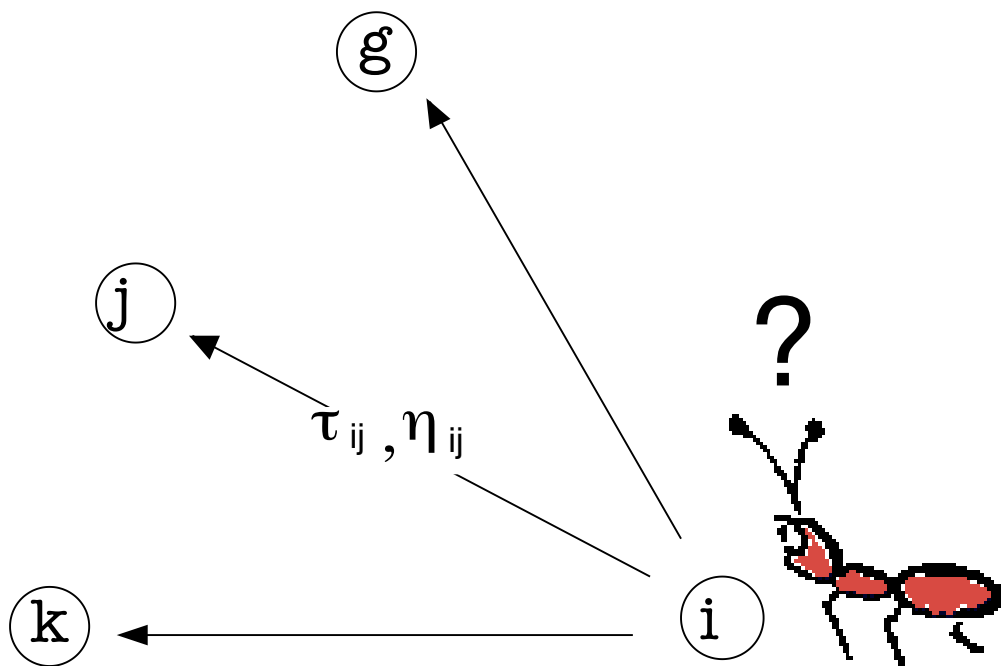
*initialise pheromone trails*

While termination criterion is not satisfied:

- generate population  $sp$  of candidate solutions  
using *subsidiary randomised constructive search*
- perform *subsidiary local search* on  $sp$
- update pheromone trails* based on  $sp$

### Note:

- ▶ In each cycle, each ant creates one candidate solution using a *constructive search procedure*.
- ▶ *Subsidiary local search* is applied to individual candidate solutions.
- ▶ All *pheromone trails* are initialised to the same value,  $\tau_0$ .
- ▶ *Pheromone update* typically comprises uniform decrease of all trail levels (*evaporation*) and increase of some trail levels based on candidate solutions obtained from construction + local search.
- ▶ *Termination criterion* can include conditions on make-up of current population, e.g., variation in solution quality or distance between individual candidate solutions.



## Example: A simple ACO algorithm for the TSP (1)

(Variant of Ant System for the TSP [Dorigo *et al.*, 1991; 1996].)

- ▶ Search space and solution set as usual (all Hamiltonian cycles in given graph  $G$ ).
- ▶ Associate pheromone trails  $\tau_{ij}$  with each edge  $(i, j)$  in  $G$ .
- ▶ Use heuristic values  $\eta_{ij} := 1/w((i, j))$ .
- ▶ Initialise all weights to a small value  $\tau_0$  (parameter).
- ▶ *Constructive search*: Each ant starts with randomly chosen vertex and iteratively extends partial round trip  $\phi$  by selecting vertex not contained in  $\phi$  with probability

$$\frac{[\tau_{ij}]^\alpha \cdot [\eta_{ij}]^\beta}{\sum_{l \in N'(i)} [\tau_{il}]^\alpha \cdot [\eta_{il}]^\beta}$$

## Example: A simple ACO algorithm for the TSP (2)

- ▶ *Subsidiary local search*: Perform iterative improvement based on standard 2-exchange neighbourhood on each candidate solution in population (until local minimum is reached).
- ▶ *Update pheromone trail levels* according to

$$\tau_{ij} := (1 - \rho) \cdot \tau_{ij} + \sum_{s' \in sp'} \Delta(i, j, s')$$

where  $\Delta(i, j, s') := 1/f(s')$  if edge  $(i, j)$  is contained in the cycle represented by  $s'$ , and 0 otherwise.

*Motivation*: Edges belonging to highest-quality candidate solutions and/or that have been used by many ants should be preferably used in subsequent constructions.

## Example: A simple ACO algorithm for the TSP (3)

- ▶ *Termination*: After fixed number of iterations (= construction + local search phases).

### Note:

- ▶ Ants can be seen as walking along edges of given graph (using memory to ensure their tours correspond to Hamiltonian cycles) and depositing pheromone to reinforce edges of tours.
- ▶ Original Ant System did not include subsidiary local search procedure (leading to worse performance compared to the algorithm presented here)

<i>ACO algorithm</i>	<i>Authors</i>	<i>Year</i>	<i>TSP</i>
Ant System	Dorigo, Maniezzo, Colorni	1991	yes
Elitist AS	Dorigo	1992	yes
Ant-Q	Gambardella & Dorigo	1995	yes
<i>Ant Colony System</i>	Dorigo & Gambardella	1996	yes
<i>MMAS</i>	Stützle & Hoos	1996	yes
Rank-based AS	Bullnheimer, Hartl, Strauss	1997	yes
ANTS	Maniezzo	1998	no
Best-Worst AS	Cordón, et al.	2000	yes
Hyper-cube ACO	Blum, Roli, Dorigo	2001	no
Population-based ACO	Guntsch, Middendorf	2002	yes
Beam-ACO	Blum	2004	no

## *MAX-MIN* Ant System

- ▶ extension of Ant System with stronger exploitation of best solutions and additional mechanism to avoid search stagnation
- ▶ *exploitation*: only the iteration-best or best-so-far ant deposit pheromone

$$\tau_{ij}(t+1) = (1 - \rho) \cdot \tau_{ij}(t) + \Delta\tau_{ij}^{best}$$

- ▶ frequently, a schedule for choosing between iteration-best and best-so-far update is used

- ▶ *stagnation avoidance*: additional limits on the feasible pheromone trails
  - ▶ for all  $\tau_{ij}(t)$  we have:  $\tau_{min} \leq \tau_{ij}(t) \leq \tau_{max}$
  - ▶ counteracts stagnation of search through aggressive pheromone update
  - ▶ heuristics for determining  $\tau_{min}$  and  $\tau_{max}$
- ▶ *stagnation avoidance 2*: occasional pheromone trail re-initialization when  $\mathcal{MMAS}$  has converged
- ▶ *increase of exploration*: pheromone values are initialized to  $\tau_{max}$  to have less pronounced differences in selection probabilities

## Ant Colony System (ACS)

Gambardella, Dorigo 1996, 1997

- ▶ pseudo-random proportional action choice rule
  - ▶ with probability  $q_0$  an ant  $k$  located at city  $i$  chooses successor city  $j$  with maximal  $\tau_{ij}(t) \cdot [\eta_{ij}]^\beta$  (*exploitation*)
  - ▶ with probability  $1 - q_0$  an ant  $k$  chooses the successor city  $j$  according to action choice rule used in Ant System (*biased exploration*)

► global pheromone update rule (*exploitation*)

- best-so-far solution  $T^{gb}$  deposits pheromone after each iteration

$$\tau_{ij}(t) = (1 - \rho) \cdot \tau_{ij}(t - 1) + \rho \cdot \Delta\tau_{ij}^{gb}(t - 1),$$

where  $\Delta\tau_{ij}^{gb}(t) = 1/L^{gb}$ .

- pheromone update only affects edges in  $T^{gb}$ !
- limited tests with iteration-best solution; however, best-so-far update is recommended

► local pheromone update rule

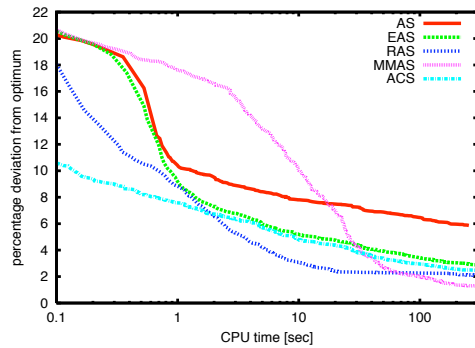
- ants “eat away” pheromone on the edges just crossed

$$\tau_{ij} = (1 - \xi) \cdot \tau_{ij} + \xi \cdot \tau_0$$

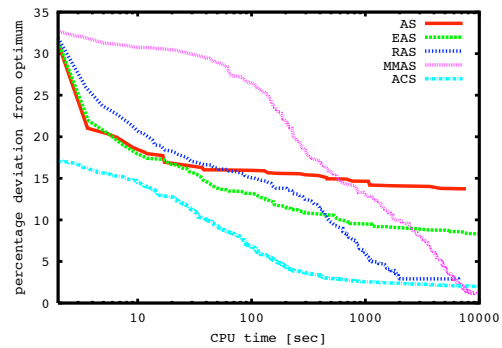
- $\tau_0$  is some small constant value
- increases exploration by reducing the desirability of frequently used edges
- in Ant-Q (predecessor of ACS):  $\tau_0 = \gamma \cdot \max_{l \in \mathcal{N}_j^k} \{\tau_{jl}\}$

## solution quality versus time

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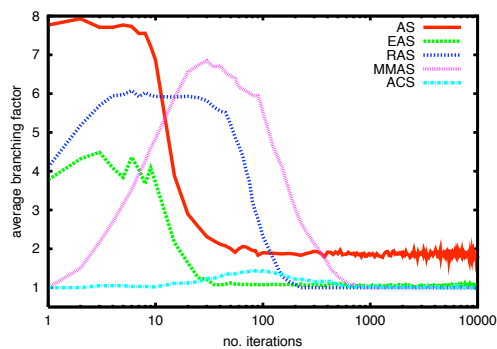
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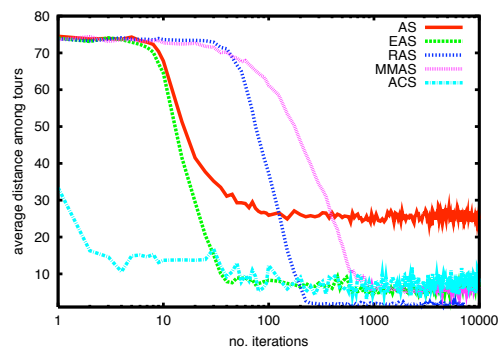
(typical parameter settings for high final solution quality)

## behavior of ACO algorithms

average  $\lambda$ -branching factor



average distance among tours

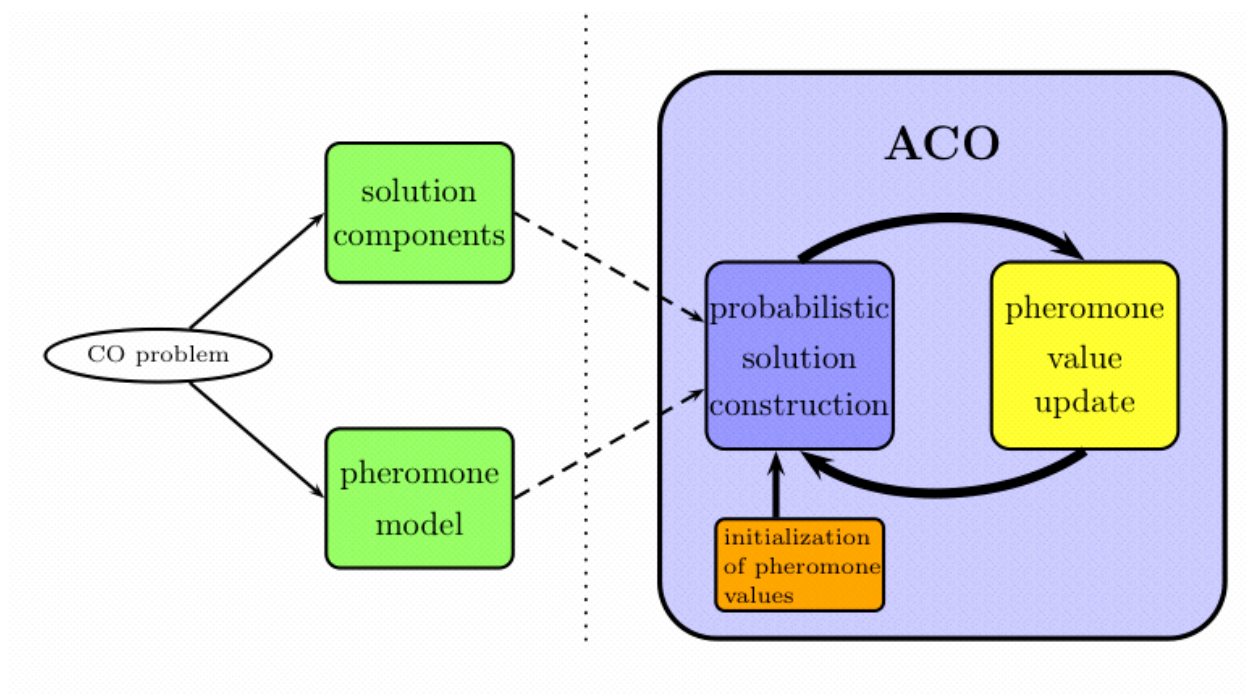


(typical parameter settings for high final solution quality)

## Enhancements:

- ▶ use of look-ahead in construction phase;
- ▶ start of solution construction from partial solutions (memory-based schemes, ideas gleaned from iterated greedy);
- ▶ combination of ants with techniques from tree search such as
  - ▶ lower bounding information
  - ▶ combination with beam search
  - ▶ constraint programming (constraint propagation)

## Applying ACO





## Ant Colony Optimisation . . .

- ▶ has been applied very successfully to a wide range of combinatorial problems, including
  - ▶ various scheduling problems,
  - ▶ various vehicle routing problems, and
  - ▶ various bio-informatics problems such as protein–ligand docking
- ▶ underlies new high-performance algorithms for *dynamic optimisation problems*, such as routing in telecommunications networks [Di Caro and Dorigo, 1998].

### Note:

A general algorithmic framework for solving static and dynamic combinatorial problems using ACO techniques is provided by the *ACO metaheuristic* [Dorigo and Di Caro, 1999; Dorigo et al., 1999].

For further details on Ant Colony Optimisation, see the course on Swarm Intelligence or the book by Dorigo and Stützle [2004].

## Evolutionary Algorithms

**Key idea:** Iteratively apply *genetic operators* *mutation*, *recombination*, *selection* to a population of candidate solutions.

### Inspired by simple model of biological evolution:

- ▶ *Mutation* introduces random variation in the genetic material of individuals.
- ▶ *Recombination* of genetic material during reproduction produces *offspring* that combines features inherited from both *parents*.
- ▶ Differences in *evolutionary fitness* lead *selection* of genetic traits ('survival of the fittest').

### Evolutionary Algorithm (EA):

determine initial population *sp*

While *termination criterion* is not satisfied:

    generate set *spr* of new candidate solutions  
        by *recombination*

    generate set *spm* of new candidate solutions  
        from *spr* and *sp* by *mutation*

*select* new population *sp* from  
        candidate solutions in *sp*, *spr*, and *spm*

**Problem:** Pure evolutionary algorithms often lack capability of sufficient *search intensification*.

**Solution:** Apply subsidiary local search after initialisation, mutation and recombination.

⇒ *Memetic Algorithms* (aka *Genetic Local Search*)

### **Memetic Algorithm (MA):**

determine initial population *sp*

perform *subsidiary local search* on *sp*

While *termination criterion* is not satisfied:

    generate set *spr* of new candidate solutions  
        by *recombination*

    perform *subsidiary local search* on *spr*

    generate set *spm* of new candidate solutions  
        from *spr* and *sp* by *mutation*

    perform *subsidiary local search* on *spm*

*select* new population *sp* from  
        candidate solutions in *sp*, *spr*, and *spm*

## Initialisation

- ▶ *Often*: independent, uninformed random picking from given search space.
- ▶ *But*: can also use multiple runs of construction heuristic.

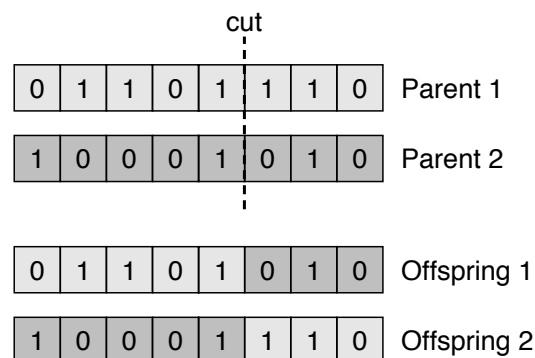
## Recombination

- ▶ Typically repeatedly selects a set of *parents* from current population and generates *offspring* candidate solutions from these by means of *recombination operator*.
- ▶ *Recombination operators* are generally based on *linear representation* of candidate solutions and piece together *offspring* from fragments of *parents*.

### Example: One-point binary crossover operator

Given two parent candidate solutions  $x_1x_2 \dots x_n$  and  $y_1y_2 \dots y_n$ :

1. choose index  $i$  from set  $\{2, \dots, n\}$  uniformly at random;
2. define offspring as  $x_1 \dots x_{i-1}y_i \dots y_n$  and  $y_1 \dots y_{i-1}x_i \dots x_n$ .



*Generalization*: two-point,  $k$ -point, uniform crossover

## Mutation

- ▶ *Goal*: Introduce relatively small perturbations in candidate solutions in current population + offspring obtained from *recombination*.
- ▶ Typically, perturbations are applied stochastically and independently to each candidate solution; amount of perturbation is controlled by *mutation rate*.
- ▶ Can also use *subsidiary selection function* to determine subset of candidate solutions to which mutation is applied.
- ▶ In the past, the role of mutation (as compared to recombination) in high-performance evolutionary algorithms has been often underestimated [Bäck, 1996].

## Selection

- ▶ *Selection for variation*: determines which of the individual candidate solutions of the current population are chosen to undergo recombination and/or mutation
- ▶ *Selection for survival*: determines population for next cycle (*generation*) of the algorithm by selecting individual candidate solutions from current population + new candidate solutions obtained from *recombination*, *mutation* (+ *subsidiary local search*).
  - ▶ *Goal*: Obtain population of high-quality solutions while maintaining *population diversity*.
- ▶ Selection is based on evaluation function (*fitness*) of candidate solutions such that better candidate solutions have a higher chance of 'surviving' the selection process.

## Selection (general)

- ▶ Many selection schemes involve probabilistic choices, using the idea that better candidate solutions have a higher probability of being chosen.
- ▶ examples
  - ▶ roulette wheel selection (probability of selecting a candidate solution  $s$  is proportional to its fitness value,  $g(s)$ )
  - ▶ tournament selection (choose best of  $k$  randomly sampled candidate solutions)
  - ▶ rank-based computation of selection probabilities
- ▶ the strength of the probabilistic bias determines the *selection pressure*

## Selection (survival)

- ▶ *generational* replacement versus *overlapping populations*; (extreme case, *steady-state selection*)
- ▶ It is often beneficial to use *elitist selection strategies*, which ensure that the best candidate solutions are always selected.
- ▶ probabilistic versus deterministic replacement
- ▶ quasi-deterministic replacement strategies implemented by classical selections schemes from evolution strategies (a particular type of EAs)
  - ▶  $\lambda$ : number offspring,  $\mu$ : number parent candidate solutions
  - ▶  $(\mu, \lambda)$  strategy: choose best  $\mu$  of  $\lambda > \mu$  offspring
  - ▶  $(\mu + \lambda)$  strategy: choose best  $\mu$  of  $\mu + \lambda$  candidate solutions

## Subsidiary local search

- ▶ Often useful and necessary for obtaining high-quality candidate solutions.
- ▶ Typically consists of selecting some or all individuals in the given population and applying an *iterative improvement procedure* to each element of this set independently.

## Example: A memetic algorithm for SAT (1)

- ▶ *Search space*: set of all truth assignments for propositional variables in given CNF formula  $F$ ; *solution set*: models of  $F$ ; use *1-flip neighbourhood relation*; *evaluation function*: number of unsatisfied clauses in  $F$ .
- ▶ *Note*: truth assignments can be naturally represented as bit strings.
- ▶ Use population of  $k$  truth assignments; *initialise* by (independent) Uninformed Random Picking.

## Example: A memetic algorithm for SAT (2)

- ▶ **Recombination:** Add offspring from  $n/2$  (independent) one-point binary crossovers on pairs of randomly selected assignments from population to current population ( $n$  = number of variables in  $F$ ).
- ▶ **Mutation:** Flip  $\mu$  randomly chosen bits of each assignment in current population (*mutation rate*  $\mu$ : parameter of the algorithm); this corresponds to  $\mu$  steps of Uninformed Random Walk; mutated individuals are added to current population.
- ▶ **Selection:** Selects the  $k$  best assignments from current population (simple *elitist selection mechanism*).

## Example: A memetic algorithm for SAT (3)

- ▶ **Subsidiary local search:** Applied after *initialisation*, *recombination* and *mutation*; performs *iterative best improvement* search on each individual assignment independently until local minimum is reached.
- ▶ **Termination:** upon finding model of  $F$  or after bound on number of cycles (*generations*) is reached.

*Note:* This algorithm does not reach state-of-the-art performance, but many variations are possible (few of which have been explored).



## Problem representation and operators

- ▶ simplest choice of candidate solution representation: bitstrings
- ▶ advantage: application of simple recombination, mutation operators
- ▶ problems with this arise in case of
  - ▶ problem constraints (e.g. set covering, graph bi-partitioning)
  - ▶ “richer” problem representations are much better suited (e.g. TSP)
- ▶ *possible solutions*
  - ▶ application of representation- (and problem-) specific recombination and mutation operators
  - ▶ application of repair mechanisms to reestablish feasibility of candidate solutions

## Memetic algorithm by Merz and Freisleben (MA-MF)

- ▶ one of the best studied MAs for the TSP
- ▶ first versions proposed in 1996 and further developed until 2001
- ▶ main characteristics
  - ▶ population initialisation by constructive search
  - ▶ exploits an effective LK implementation
  - ▶ specialised recombination operator
  - ▶ restart operators in case the search is deemed to stagnate
  - ▶ standard selection and mutation operators

## MA-MF: population initialisation

- ▶ each individual of initial population constructed by a randomised variant of the greedy heuristic

Step 1: choose  $n/4$  edges by the following two steps

- ▶ select a vertex  $v \in V$  uniformly at random among those that are not yet in partial tour
- ▶ insert shortest (second-shortest) feasible edge incident to  $v$  with a probability of  $2/3$  ( $1/3$ )

Step 2: complete tour using the greedy heuristic

- ▶ locally optimise initial tours by LK

## MA-MF: recombination

- ▶ various specialised crossover operators examined (distance-preserving crossover, greedy crossover)
- ▶ crossover operators generate feasible offspring
- ▶ best performance by greedy crossover that borrows ideas from greedy heuristic
- ▶ one offspring is generated from two parents:
  1. copy fraction of  $p_e$  common edges to offspring
  2. add fraction of  $p_n$  new short edges not contained in any of the parents
  3. add fraction of  $p_c$  shortest edges from parents
  4. complete tour by greedy heuristic
- ▶ best performance for  $p_e = 1$ ;  $\mu/2$  pairs of tours are chosen uniformly at random from population for recombination

## MA-MF: mutation, selection, restart, results

- ▶ *mutation* by (usual) double-bridge move
- ▶ *selection* done by usual  $(\mu + \lambda)$  strategy
  - ▶  $\mu$ : population size,  $\lambda$ : number of new offspring generated
  - ▶ select  $\mu$  lowest weight tours among  $\mu + \lambda$  current tours for next iteration
  - ▶ take care that no duplicate tours occur in population
- ▶ *partial restart* by strong mutation
  - ▶ if average distance is below 10 or did not change for 30 iterations, apply random  $k$ -exchange move ( $k = 0.1 \cdot n$ ) plus local search to all individuals except population-best one
- ▶ *results*: high solution quality reachable, though not fully competitive with state-of-the-art ILS algorithms for TSP

## Memetic algorithm by Walters (MA-W)

- ▶ differs in many aspects from other MAs for the TSP
- ▶ main differences concern
  - ▶ solution representation by nearest neighbour indexing instead of permutation representation
  - ▶ usage of general-purpose recombination operators that may generate infeasible offspring
  - ▶ repair mechanism is used to restore valid tours from infeasible offspring
  - ▶ uses "only" a 3-opt algorithm as subsidiary local search

## MA-W: solution representation, initialisation, mutation

- ▶ *solution representation* through nearest neighbour indexing
  - ▶ tour  $p$  represented as vector  $s := (s_1, \dots, s_n)$  such that  $s_i = k$  if, and only if, the successor of vertex  $u_i$  in  $p$  is  $k$ th nearest neighbour of  $u_i$
  - ▶ leads, however, to some redundancies for symmetric TSPs
- ▶ *population initialisation* by choosing randomly nearest neighbour indices
  - ▶ three nearest neighbours selected with probability of 0.45, 0.25, 0.15, respectively
  - ▶ in remaining cases index between four and ten chosen uniformly at random
- ▶ *mutation* modifies nearest neighbour indices of randomly chosen vertices according to same probability distribution

## MA-W: recombination, repair mechanism, results

- ▶ *recombination* is based on a slight variation of standard two-point crossover operator
- ▶ infeasible candidate solutions from crossover and mutation are repaired
- ▶ *repair mechanism* tries to preserve as many edges as possible and replaces an edge  $e$  by an edge  $e'$  such that  $|w(e) - w(e')|$  is minimal
- ▶ *results* are interesting considering that "only" 3-opt was used as subsidiary local search; however, worse than state-of-the-art ILS algorithms

## Tour merging

- ▶ can be seen as an extreme case of MAs
- ▶ exploits information collected by high-quality solutions from various ILS runs in a two phases approach
- ▶ *phase one*
  - ▶ generate a set  $T$  of very high quality tours for  $G = (V, E, w)$
  - ▶ define subgraph  $G' = (V, E', w')$ , where  $E'$  contains all edges in at least one  $t \in T$  and  $w'$  is original  $w$  restricted to  $E'$
- ▶ *phase two*
  - ▶ determine optimal tour in  $G'$
  - ▶ *Note:* general-purpose or specialised algorithm that exploit characteristics of  $T$  are applicable
- ▶ very high quality solutions can be obtained
  - ▶ optimal solution to TSPLIB instance d15112 in 22 days on a 500 MHz Alpha processor
  - ▶ new best-known solutions to instances brd14051 and d18512

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## Types of evolutionary algorithms (1)

- ▶ *Genetic Algorithms (GAs)* [Holland, 1975; Goldberg, 1989]:
  - ▶ have been applied to a very broad range of (mostly discrete) combinatorial problems;
  - ▶ often encode candidate solutions as bit strings of fixed length, which is now known to be disadvantageous for combinatorial problems such as the TSP.

*Note:* There are some interesting theoretical results for GAs (e.g., *Schema Theorem*), but – as for SA – their practical relevance is rather limited.

## Types of evolutionary algorithms (2)

- ▶ *Evolution Strategies* [Rechenberg, 1973; Schwefel, 1981]:
  - ▶ originally developed for (continuous) numerical optimisation problems;
  - ▶ operate on more natural representations of candidate solutions;
  - ▶ use *self-adaptation* of perturbation strength achieved by *mutation*;
  - ▶ typically use *elitist deterministic selection*.
- ▶ *Evolutionary Programming* [Fogel *et al.*, 1966]:
  - ▶ similar to Evolution Strategies (developed independently), but typically does not make use of *recombination* and uses *stochastic selection* based on *tournament mechanisms*.