

Hybrid Metaheuristics (Vienna 2022)

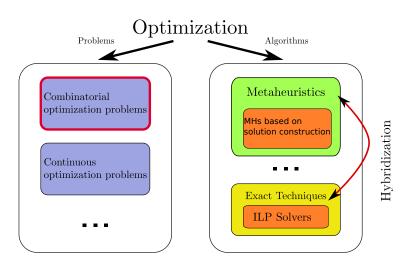
©Christian Blum

Artificial Intelligence Research Institute (IIIA-CSIC)





Artificial Intelligence Research Institute (IIIA-CSIC)



Exact methods for combinatorial optimization

- Exhaustive search (not practical)
- Mathematical programming
 - Branch & bound (B&B)
 - Branch & cut (B&B + cutting planes to tighten LP relaxations)
 - Branch & price (hybrid between B&B and column generation)
- Dynamic programming
- Constraint programming

Generic branch & bound



Artificial Intelligence Research Institute (IIIA-CSIC)

B&B, general description. Clarification on the board!

- Branch & Bound (B&B) is a tree search algorithm
- Each node of the search tree corresponds to a sub-problem
- B&B make use of a strategy for the sub-division of sub-problems (branching rule)
- B&B uses bounding information in order to discard sub-problems and prove optimality
- Optionally uses a heuristic

Generic branch & bound



Artificial Intelligence Research Institute (IIIA-CSIC)

Pseudo code

```
1: B := \infty
 2: if heuristic available then s := ApplyHeuristic(); B := f(s); s_{bsf} := s
   Initialize a queue Q containing only the root node of the search tree
 4: while Q is not empty do
      Choose a node N from the queue Q (and remove N from Q)
 5:
      if N contains a single solution s' then
 6:
         if f(s') < B then B := f(s') and s_{bsf} := s' end if
 7:
      else
 8:
         Use the branching rule to produce a set of sub-problems N_{\text{sub}}
 9:
         from N
         for all N_i \in N_{\text{sub}} do
10:
           if LB(N_i) \leq B then add N_i to Q end if
11:
         end for
12:
      end if
13:
```

14: end while

Generic branch & bound



Artificial Intelligence Research Institute (IIIA-CSIC)

Different ways to handle queue Q

- Last-in-first-out (LIFO): results in a depth-first algorithm
- First-in-first-out (FIFO): results in a breath-first algorithm
- When the ordering in queue Q depends on LB(): results in a best-first algorithm

Note

When no heuristic is available, the FIFO variant is preferable.

Dynamic programming (DP)



Artificial Intelligence Research Institute (IIIA-CSIC)

How does it work?

- Divide the given problem into sub-problems
- 2 Combine solutions of already solved sub-problems to solutions to bigger sub-problems until a solution for the original problem is obtained

Required properties of the problem

- 1 Optimal substructure: optimal solution to the problem must contain optimal solutions to sub-problems
- 2 Overlapping sub-problems: solutions to high-level sub-problems reuse lower level sub-problems
- **Size of the sub-problem space:** should be of moderate size (polynomial)

DP example: LCS problem



Artificial Intelligence Research Institute (IIIA-CSIC)

Definition: longest common subsequence (LCS) problem

- **Given:** input strings x and y of length |x| = n y |y| = m
- $x = x[1] \dots x[n], y = y[1] \dots y[m]$
- Let x_i denote the prefix of x until position i
- **Example:** if x = BANANA then $x_3 = BAN$
- Let LCS(x, y) denote the LCS between x and y

Note

- 1 Case 1: $x[n] = y[m] LCS(x, y) = LCS(x_{n-1}, y_{m-1}) + x[n]$
- 2 Case 2: $x[n] \neq y[m]$
 - Sub-case 2.1: if LCS(x, y) ends with x[n]. Then: $LCS(x, y) = LCS(x, y_{m-1})$
 - Sub-case 2.2: if LCS(x, y) does not end with x[n]. Then: $LCS(x, y) = LCS(x_{n-1}, y_m)$



Artificial Intelligence Research Institute (IIIA-CSIC)

Resulting DP formula

For any $i \in \{0, 1, \dots, n\}$ and $j \in \{0, 1, \dots, m\}$

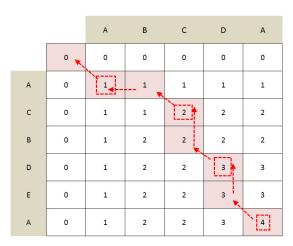
$$LCS(x_i, y_j) = \begin{cases} \epsilon & \text{(empty string)} & \text{if } i = 0 \text{ or } j = 0 \\ LCS(x_{i-1}, y_{j-1}) + x[i] & \text{if } x[i] = y[j] \\ \max(LCS(x_i, y_{j-1}), LCS(x_{i-1}, y_j)) & \text{if } x[i] \neq y[j] \end{cases}$$

DP example: LCS problem



Artificial Intelligence Research Institute (IIIA-CSIC)

Application of the DP formula



LCS - "ACDA"

Constraint programming (CP)



Artificial Intelligence Research Institute (IIIA-CSIC)

Characterization of constraint programming (CP)

CP is a computational system based on constraints

How does it work?

- Phase 1:
 - Express the CO problem in terms of a discrete problem (variables + domains)
 - Define constraints among the variables ("post constraints")
 - The constraint solver tries to reduce the variable domains (propagation)
 - ... before solution construction
 - ... after solution construction
- Phase 2: Labeling
 - Search through the remaining search tree
 - Possibly add (post) additional constraints



Artificial Intelligence Research Institute (IIIA-CSIC)

Simple example

 $\textbf{minimize}\ f(X,Y,Z)\mapsto \mathbb{R}$

suject to

$$X \in \{1, \dots, 8\}$$

$$Y, Z \in \{1, \dots, 10\}$$

$$X \neq 7, Z \neq 2$$

$$X - Z = 3Y$$

Constraint propagation (step 1)

- Use $X \neq 7$ and $Z \neq 2$
 - 1 $X \in \{1, \dots, 6, 8\}$
 - **2** $Z \in \{1, 3, \dots, 10\}$

CP: domain reduction (example)



Artificial Intelligence Research Institute (IIIA-CSIC)

Constraint propagation (step 2)

- Make use of X Z = 3Y
 - 1 Because of the domains of X and Z: X Z < 8
 - $|2\rangle \Rightarrow 3Y < 8$
 - $|3| \Rightarrow Y < 2$
 - **4** \Rightarrow *Y* \in {1, 2}

Constraint propatation (step 3)

- Use again X Z = 3Y
 - 1 Because of the reduced domain of $Y: 3Y \ge 3$
 - $\mathbf{2} \Rightarrow X Z \geq 3$
 - 3 $\Rightarrow X \in \{4,5,6,8\} \text{ y } Z \in \{1,3,4,5\}$

Hybrid metaheuristics: topics



Artificial Intelligence Research Institute (IIIA-CSIC)

- Hybrid Metaheuristics (HMs)
 - Definition
 - Clasification
- Examples
 - Metaheuristics with other metaheuristics (ILS)
 - Metaheuristics with constraint programming (ACO)
 - Metaheuristics with tree search (VNS)
 - Metaheuristics with problem relaxation (TS)
 - Metaheuristics with dynamic programming (EC)
- New algorithms/approaches from my group: CMSA y ACO_neg

Questions?



Artificial Intelligence Research Institute (IIIA-CSIC)



MHs: no new idea since 2005!



Artificial Intelligence Research Institute (IIIA-CSIC)

Important metaheuristics, year of introduction

Simulated Annealing (SA)	[Kirkpatrick, 1983]
/	F

Tabu Search (TS) [Glover, 1986]

Genetic and Evolutionary Computation (EC) [Goldberg, 1989]
 Ant Colony Optimization (ACO) [Dorigo, 1992]

Ant Colony Optimization (ACO) [Dorigo, 1992]
 Greedy Rand. Adaptive Search Procedure (GRASP) [Resende, 1995]

Particle Swarm Optimiation (PSO) [Eberhart, Kennedy, 1995]

Guided Local Search (GLS) [Voudouris, 1997]

■ Iterated Local Search (ILS) [Stützle, 1999]

■ Variable Neighborhood Search (VNS) [Mladenović, 1999]

Artificial Bee Colony (ABC) [Karaboga, 2005]

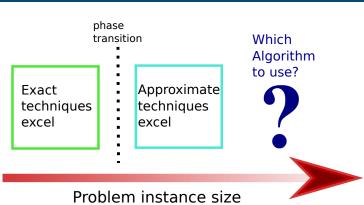
Note

No essentially new metaheuristics were introduced after 2005!!!

Hybrid metaheuristics: reasons for being



Artificial Intelligence Research Institute (IIIA-CSIC)



Note

Hybrid algorithms that take advantage of synergies between exact algorithms and approximate algorithms often excel for large-scale problems.

Hybrid MHs: characterization



Artificial Intelligence Research Institute (IIIA-CSIC)

What exactly is a hybrid metaheuristic?

Problem: this is not well-defined!

Possible characterization

- Hybrid MHs are techniques that result from the combination of a metaheuristic with other techniques for optimization
- Options for such other techniques:
 - Metaheuristics
 - Branch & bound
 - Dynamic programming
 - Integer linear programming (ILP)

Hybrid MHs: history



Artificial Intelligence Research Institute (IIIA-CSIC)

Pathway towards hybrid MHs

- For a long time the different optimization communities co-existed quite isolated
- Hybrid approaches were developed already early, but only sporadically
- Only since about 20 years the published body of research grows significantly significativa:
 - 1 1999: first celebration of the CP-AI-OR conference
 - 2 2004: first celebration of the **Hybrid Metaheuristics (HM)** workshop
 - 3 2006: first celebration of the Matheuristics Workshops

Consequence

Nowadays the term hybrid metaheuristic identifies a new line of research.

Hybrid MHs: classification



Artificial Intelligence Research Institute (IIIA-CSIC)

Articles about the classification of hybrid MHs

- C. Cotta. A study of hybridisation techniques and their application to the design of evolutionary algorithms, AI Communications, 11(3-4):223-224, 1998
- E. Talbi. **A taxonomy of hybrid metheuristics**, *Journal of Heuristics*, 8(5):541–565, 2002
- G. Raidl. A unified view on hybrid metaheuristics, In: Proceedings of HM 2006, volume 4030, Springer LNCS, pages 1–112, 2006
- E.-G. Talbi, ed. Hybrid metaheuristics, Vol. 434 of Studies in Computational Intelligence, Springer, 2013
- C. Blum and G. Raidl. Hybrid Metaheuristics Powerful Tools for Optimization, Springer, 2016

Different angles for the classification



Artificial Intelligence Research Institute (IIIA-CSIC)

Concerning the types of algorithms that are combined

- Metaheuristics with other metaheuristics. Examples:
 - 1 Use of neighborhood-based MHs within population-based MHs
 - 2 Multi-level frameworks
- Metaheuristics with problem-specific techniques. Examples:
 - 1 Continuous optimization: use of gradient-based methods
 - 2 Simulations for approximating the objective function
- Metaheuristics with other AI/OR techniques. Examples:
 - 1 Large neighborhood search (LNS)
 - 2 Combinations of metaheuristics with constraint programming
- Metaheuristics with a human interactor

Different angles for the classification



Artificial Intelligence Research Institute (IIIA-CSIC)

Depth/level of the hybridization

- High-level: weak coupling
 - 1 Algorithms retain their own identities
 - 2 No direct relationship of the internal workings of the algorithms
 - 3 Interaction over a well-defined interface
- Low-level: strong coupling
 - 1 Algorithms strongly depend on each other
 - 2 Individual components or functions are exchanged

Different angles for the classification



Artificial Intelligence Research Institute (IIIA-CSIC)

What is the control strategy?

Collaborative

- 1 Homogeneous approaches: several instances of the same algorithm
- 2 Heterogeneous approaches: for example, A-Teams

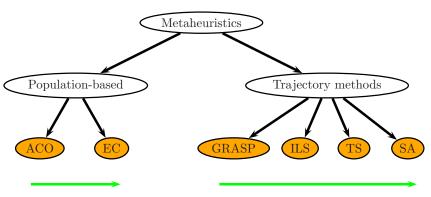
Integrative

- 1 Solution merging (optimal crossover)
- 2 Decoder-based approaches
- 3 Large neighborhood search (LNS)
- 4 Using metaheuristics for finding good upper bounds in branch & bound

Characteristics of different MHs



Artificial Intelligence Research Institute (IIIA-CSIC)



Decreasing use of constructive elements

Decreasing use of constructive elements

- Advantage of population-based methods: diversification
- Advantage of trajectory methods: intensification

Consequences for hybridization



Artificial Intelligence Research Institute (IIIA-CSIC)

Consequence

Most MH/MH hybrids incorporate trajectory methods into population-based techniques

Examples

- Application of local search to solutions constructed by ACO
- Application of local search to individuals in evolutionary algorithms (memetic algorithms)
- Population-based extension of iterated local search (ILS)
- Multi-level techniques

Iterated local search (ILS)



Artificial Intelligence Research Institute (IIIA-CSIC)

Pseudo code

```
s_0 \leftarrow \mathsf{GenerateInitialSolution}()
```

 $s^* \leftarrow \mathsf{LocalSearch}(s_0)$

while termination conditions not met do

 $s' \leftarrow \mathsf{Perturbation}(s^*)$

 $s^{*\prime} \leftarrow \mathsf{LocalSearch}(s^\prime)$

 $s^* \leftarrow \mathsf{AcceptanceCriterion}(s^*, s^{*\prime})$

end while

output: best solution found

Key components

- Perturbation mechanism
- Local search



990

27

Artificial Intelligence Research Institute (IIIA-CSIC)

Pseudo code

- 1: $P \leftarrow \text{GenerateInitialPopulation}(n)$
- 2: Apply LocalSearch() to all $s \in P$
- 3: while termination conditions not met do
- 4: $P' \leftarrow P$
- 5: **for** all $s \in P$ **do**
- 6: $s' \leftarrow \text{Perturbation}(s)$
- 7: $\hat{s'} \leftarrow \text{LocalSearch}(s')$
- $P' \leftarrow P' \cup \{\hat{s'}\}$
- 9: end for
- 10: $P \leftarrow \text{Best } n \text{ solutions from } P'$
- 11: end while

¹T. Stützle. **Iterated local search for the quadratic assignment problem**, European Journal of Operational Research, 174(3):1529−1539, 2⊕06 ← ■ → ← ■ →

Multi-level techniques



Artificial Intelligence Research Institute (IIIA-CSIC)

Articles

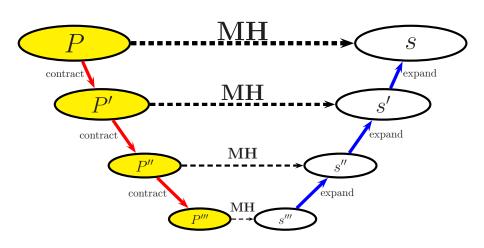
- C. Walshaw. Multilevel refinement for combinatorial optimisation, Annals of Operations Research, 131:325–372, 2004
- C. Walshaw. Multilevel refinement for combinatorial optimisation: boosting metaheuristic performance, In: Hybrid Metaheuristics—An Emerging Approach to Optimization, volume 114 of Studies in Computational Intelligence, pages 261–289, Springer Verlag, Berlin, Germany, 2008

General idea

- <u>First:</u> Iterative coarsening of the original problem instance
- Then: Find a solution to the coarsest level
- Finally: Iteratively refine this solution at each level



Artificial Intelligence Research Institute (IIIA-CSIC)



Multi-level techniques: TSP example



Artificial Intelligence Research Institute (IIIA-CSIC)

Example: on the board!

Application of the multi-level framework to the TSP. Here are some references to interesting applications. ^{abc}

^aC. Walshaw. **A multilevel approach to the travelling salesman problem**, *Operations Research*, 50(5):862–877, 2002

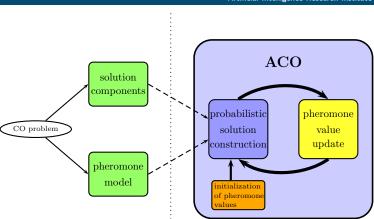
^bT. G. Crainic, Y. Li, and M. Toulouse. **A first multilevel cooperative algorithm for capacitated multicommodity network design**, *Computers & Operations Research*, 33(9):2602–2622, 2006

^cP. Lin, M. A. Contreras, R. Dai, and J. Zhang. **A multilevel ACO** approach for solving forest transportation planning problems with environmental constraints, *Swarm and Evolutionary Computation*, 28:78–87, 2016



31

Artificial Intelligence Research Institute (IIIA-CSIC)



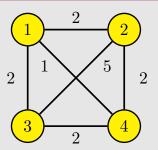
Note

As any other technique based on solution construction, ACO can be seen as a tree search algorithm



Artificial Intelligence Research Institute (IIIA-CSIC)

Example TSP instance



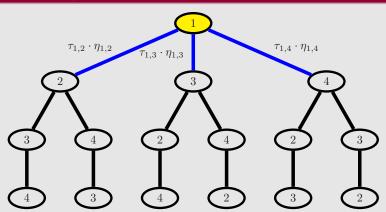
Solution construction mechanism

We will use the nearest-neighbor heuristics, starting every solution construction in city 1.



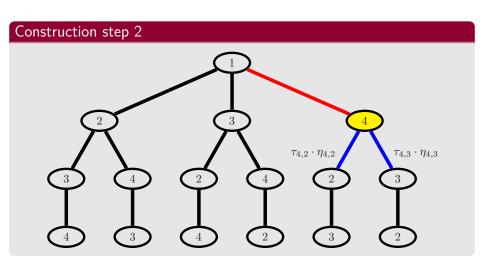
Artificial Intelligence Research Institute (IIIA-CSIC)

Construction step 1





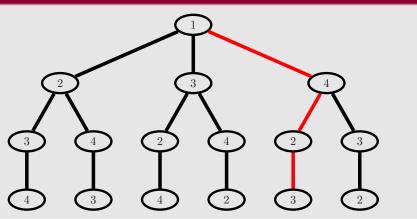
Artificial Intelligence Research Institute (IIIA-CSIC)





Artificial Intelligence Research Institute (IIIA-CSIC)

Final solution constructed



Hybrid between ACO and CP

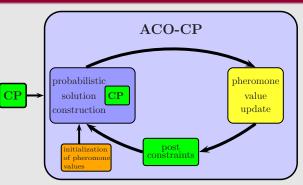


Artificial Intelligence Research Institute (IIIA-CSIC)

General idea

- Successively reduce the variable domains by constraint propagation
- Let ACO search the reduced search tree

Graphical illustration



Hybrid between ACO and CP



Artificial Intelligence Research Institute (IIIA-CSIC)

Reasons for the benefits of such a hybrid

- Advantage of ACO: good in finding high quality solutions for moderately constrained problems
- Advantage of CP: good in finding feasible solutions for highly constrained problems
- Advantage of ACO-CP: good with intermediate number of feasible solutions factibles.^a

Problems

- Constraint propagation takes a lot of time
- Moreover: constraint propagation is repeated many times

^aB. Meyer and A. Ernst. **Integrating ACO and Constraint Propagation**, In: *Proceedings of ANTS 2004*, volume 3172 of Springer LNCS, pages 166–177, 2004

Essential information

- Large neighborhood search (LNS) is known as one of the classical hybrid algorithms
- One of the first LNS applications deals with partitioning problems^a
- A good recent survey can be found in^b

^aAhuja, R. K., Orlin, J. B., & Sharma, D. Very largescale neighborhood search. International Transactions in Operational Research, 7(45), 301-317, 2000.

^bDavid Pisinger, Stefan Ropke. Large Neighborhood Search, Handbook of Metaheuristics, International Series in Operations Research & Management Science Volume 272, 2019, pp 99-128

LNS: description (1)



Artificial Intelligence Research Institute (IIIA-CSIC)

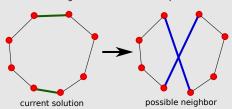
LNS is an algorithm based on local search

- Crucial for any local search method: Choice of a neighborhood
- **Usual in standard metaheuristics:** rather small neighborhoods, that is, each solution has a limited number of neighbors

Example of a small TSP neighborhood: 2-opt

Number of neighbors: $O(n^2)$

Traveling Salesman Problem: 2-opt move



LNS: description (3)



41

Artificial Intelligence Research Institute (IIIA-CSIC)

Trade-off in local search

- Small neighborhoods:
 - 1 Advantage: it is fast to find an improving neighbor (if any)
 - 2 Disadvantage: the average quality of the local minima is low
- Large-scale neighborhoods:
 - 1 Advantage: the average quality of the local minima is high
 - 2 **Disadvantage:** finding an improving neighbor might itself be NP-hard due to the size of the neighborhood

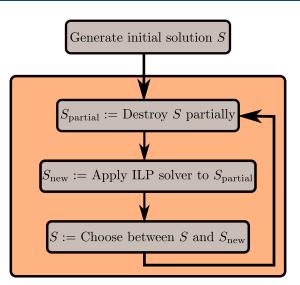
Ways to generate and explore large neighborhoods

- There are different ways to generate large neighborhoods. The most common way is to partially destroy an incumbent solution, with a subsequent reconstruction
- Large neighborhoods can be explored heuristically
- But also by making use of exact methods: for example, ILP solvers

Basic LNS based on solution destruction



Artificial Intelligence Research Institute (IIIA-CSIC)



Crucial aspects of LNS



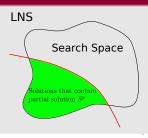
43

Artificial Intelligence Research Institute (IIIA-CSIC)

Coniderations

- **Important:** The application of an exact method in order to find the best solution containing a partial solution S_{parcial} means applying the exact method to a reduced search space.
- Consequence: In this way the exact method can be applied to larger problem instances.

Graphical illustration



LNS example: MWDS problem



Artificial Intelligence Research Institute (IIIA-CSIC)

Minimum weight dominating set (MWDS) problem

- Given: an undirected graph G = (V, E); each $v_i \in V$ has a weight $w(v_i) \ge 0$
- Valid solutions: Each $S \subseteq V$ is a valid solution, if and only if $\forall v_i \in V \colon N[v_i] \cap S \neq \emptyset$
- **Optimization objective:** finding a solution S^* that minimizes $f(S^*) := \sum_{v_i \in S^*} w(v_i)$



Given graph G



A valid solution



The optimal solution

LNS example: ILP is used as solver



Artificial Intelligence Research Institute (IIIA-CSIC)

ILP model

$$\begin{array}{ll} \min & \sum_{v_i \in V} x_i w(v_i) \\ \text{subject to} & x_i + \sum_{v_j \in N(v_i)} x_j \geq 1 \\ & x_i \in \{0,1\} \end{array} \qquad \forall \ v_i \in V$$

Note

- In this ILP: the number of variables and constraints is linear in the problem parameters
- \blacksquare How to find the best solution that contains $\mathcal{S}_{\mathrm{parcial}}?$ Add the following constraints to the ILP:

$$x_i = 1$$
 for all $v_i \in S_{\text{parcial}}$

LNS example: greedy heuristic

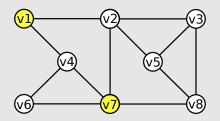


Artificial Intelligence Research Institute (IIIA-CSIC)

Definitions

- V_{cov} : the set of covered nodes (w.r.t. a partial solution))
- $\frac{d(v|V_{cov}):}{\text{nodes}} \frac{\text{current degree}}{\text{of node } v \text{ (not considering already covered}}$

Graphical illustration



$$S = \{v_1, v_7\}, \quad V_{\text{cov}} = \{v_1, v_2, v_4, v_6, v_7, v_8\}, \quad d(v_3|V_{\text{cov}}) = 1$$



Pseudo code of GREEDY

- 1: **input:** undirected graph G = (V, E) with node weights
- 2: $S := \emptyset$
- 3: $V_{cov} := \emptyset$
- 4: while $V_{cov} \neq V$ do

5:
$$v^* := \operatorname{argmax}_{v \in V \setminus V_{cov}} \left\{ \frac{d(v|V_{cov})}{w(v)} \right\}$$

- 6: $S := S \cup \{v^*\}$
- 7: $V_{\text{cov}} := V_{\text{cov}} \cup N[v^*]$
- 8: end while
- 9: **output:** *S*

LNS example: partial sol. destruction



Artificial Intelligence Research Institute (IIIA-CSIC)

Partial destruction: standard method

Remove a certain percentage $perc_{dest}$ of the nodes of S

How to select the nodes to be removed?

- **Destruction** $type_{dest} = random$: random selection of nodes
- **Destruction** $type_{dest} = biased$: selection biased by the greedy function

Choosing a value for percdest

- Dynamic scheme for choosing from $[perc_{dest}^{I}, perc_{dest}^{u}]$
- Initially $perc_{dest} := perc_{dest}^{I}$
- When no improving solution is found: $perc_{dest} := perc_{dest} + 5$
- When an improving solution is found or the upper bound is reached: $perc_{dest}^{l} := perc_{dest}^{l}$

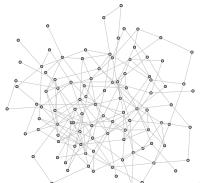
LNS example: MWDS instances



Artificial Intelligence Research Institute (IIIA-CSIC)

Problem instances used for the experiments

- **Random** graphs with $|V| = \{100, 1000, 5000, 10000\}$ nodes
- Different edge probabilities e_p (low, medium, high):
 - For |V| = 100: $e_p \in \{0.03, 0.04, 0.05\}$
 - For |V| > 100: $e_p \in \{0.01, 0.03, 0.05\}$



LNS example: parameter tuning



Artificial Intelligence Research Institute (IIIA-CSIC)

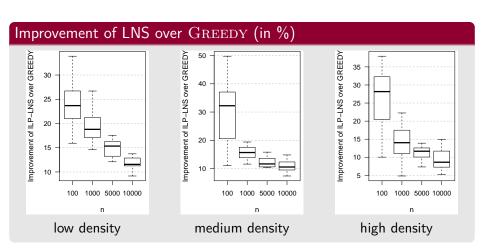
Algorithm parameters and their domains

- *type*_{dest} may be random or biased
- Upper and lower bounds (percdest, percdest) for the destruction percentage:
 - 1 (X, X) where $X \in \{10, 20, 30, 40, 50, 60, 70, 80, 90\}$
 - **2** $(X, Y) \in \{(10, 30), (10, 50), (30, 50), (30, 70)\}$
- \mathbf{t}_{max} : maximum CPU time for the ILP solver at each LNS iteration

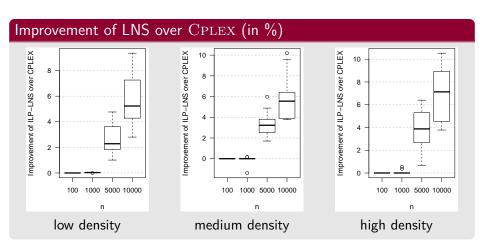
Parameter values chosen by irace

V	type _{dest}	$(perc_{dest}^{l}, perc_{dest}^{u})$	t _{max}
100	1	(60, 60)	2.0
1000	0	(90, 90)	10.0
5000	1	(50, 50)	5.0
10000	1	(40, 40)	10.0









2nd LNS example: optimization problem



Artificial Intelligence Research Institute (IIIA-CSIC)

Biological background

- Given: a set of haplotype sequences from a population of individuals
- **Goal:** study the evolutionary history of the chosen individuals
- Important for the discovery of the genetic basis of complex diseases

In case the population has evolved from a relatively small set of founders, the evolutionary history can be studied by trying to reconstruct the haplotype sequences from founder fragments

Problem

Generally, neither the founder sequences nor their number are known

2nd LNS example: optimization problem



Artificial Intelligence Research Institute (IIIA-CSIC)

The Founder Sequence Reconstruction (FSRP) problem

- Given: a set of m recombinants $C = \{C_1, ..., C_m\}$, where C_i is a binary string of length n
- Candidate solution: a set of k founders $\mathcal{F} = \{F_1, \dots, F_k\}$, where F_j is a binary string of length n
- lacksquare is a valid solution if $\mathcal C$ can be reconstructed from $\mathcal F$
- This is the case when each $C_i \in \mathcal{C}$ can be **decomposed** into a sequence of $p_i \leq n$ fragments $(Fr_{i1}Fr_{i2} \dots Fr_{ip_i})$ such that each fragment Fr_{ij} appears at the same position in at least one of the founders
- Given \mathcal{F} , a **minimal decomposition**, which is characterized by a minimal number $f(\mathcal{F}) := \sum_{i=1}^{n} p_i n$ of breakpoints, can be derived in polynomial time.
- **Optimization objective:** given k, find a valid solution \mathcal{F}^* that minimizes $f(\cdot)$.

2nd LNS example: optimization problem



Artificial Intelligence Research Institute (IIIA-CSIC)

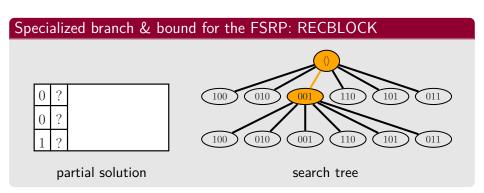
Small example instance		
1 1 0 1 1 0 1		b b b b b c c
$1\; 0\; 1\; 0\; 0\; 0\; 1$	$0\ 1\ 1\ 0\ 1\ 0\ 0$	$\begin{smallmatrix} c & c & c & c & c & c & c \end{smallmatrix}$
0 1 1 1 1 1 1	$1\ 1\ 0\ 1\ 1\ 1\ 1$	a a a b b b b
0 1 1 0 1 0 0	$1\; 0\; 1\; 0\; 0\; 0\; 1$	aaaaaa
$1\; 1\; 0\; 0\; 0\; 1\; 1$		b b b c c b b
Recombinants \mathcal{C}	Founders \mathcal{F}	Reconstruction

2nd LNS example: exact technique



56

Artificial Intelligence Research Institute (IIIA-CSIC)



2

²Wu, Y., Gusfield, D. Improved algorithms for inferring the minimum mosaic of a set of recombinants. In: *Proceedings of CPM 2007*, Volume 4580 of LNCS, Springer Verlag, Berlin (2007), pages 150–161

2nd LNS example: exact technique



Artificial Intelligence Research Institute (IIIA-CSIC)

Observation

Given some fixed founders, RECBLOCK can be used to obtain the optimal setting for the remaining founders

Example: 4 fixed founders $\{1, 2, 4, 7\}$, and 3 missing founders $\{3, 5, 6\}$



Observation

VND is a heuristic version of variable neighborhood search (VNS)

Pseudo code

- 1: **input:** a solution s, r_{max} neighborhoods
- 2: r := 1
- 3: while $r \leq r_{\text{max}}$ do
- 4: $s' := \text{ChooseBestNeighbor}(s, \mathcal{N}_r)$
- 5: **if** f(s') < f(s) **then**
- 6: s := s', r := 1
- 7: **else**
- 8: r := r + 1
- 9: end if
- 10: end while
- 11: **output:** an optimization solution *s*

2nd LNS example: the algorithm



Artificial Intelligence Research Institute (IIIA-CSIC)

LNS (based on VND) for the FRSP

```
1: input: a solution s, parameter x < k
2: r := 1
3: while r < x do
   \hat{s} := PartialDestruction(s, r)
5: s' := RECBLOCK(\hat{s})
6: if f(s') < f(s) then
7:
   s := s'
8.
    r := 1
    else
9.
        if termination conditions not met then r := r + 1
10:
     end if
11:
     if r = x + 1 then r := 1 end if
12.
13: end while
14: output: an improved solution s
```

Example: hybridization based on relaxation



Artificial Intelligence Research Institute (IIIA-CSIC)

Note

Problem relaxations can be obtained (among others) by ...

- Simplifying the constraints of an ILP model
- Dropping some constraints from an ILP model
 - **Example:** integrality constraints
- Removing some constraints and adding them as penalties to the objective function

Example: Lagrangian relaxation

Use of relaxations

- As bounds for branch & bound algorithms
- As approximation for integer solutions
- As heuristic information for solution construction



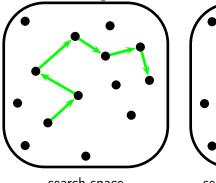
Reminder: tabu search (TS)



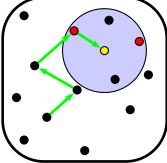
Artificial Intelligence Research Institute (IIIA-CSIC)

Main characteristics

- Use of tabu lists for storing solution features
- Note: tabu lists are used to avoid going back to already visited solutions



search space



selection of a neighbor



Specific Reference

M. Vasquez and Y. Vimont. **Improved results on the 0–1** multidimensional knapsack problem. *European Journal of Operational Research*, 165(1):70–81, 2005

Characteristics of this hybrid method

- Collaborative hybridization approach
- The algorithm makes use of two phases:
 - 1 Phase 1: problem relaxation is used to produce a bunch of promising solutions
 - 2 Phase 2: tabu search is used to search around these solutions

Reminder: MDKP problem



Artificial Intelligence Research Institute (IIIA-CSIC)

Multidimensional Knapsack Problem (MDKP) problem

- Given:
 - *n* objects, each object *i* has a profit *c_i*
 - \blacksquare m resources, each resource j has a capacity b_i
 - Each object i has a requirement a_{ij} concerning resource j
- Valid solutions: every subset of the objects such that the capacity constraints of the resources are respected
- Optimization objective: maximizing the sum of the profits of the chosen objects

ILP model



Main ideas of phase 1 of hybrid TS

- Dropping the integrality constraints of the ILP model
- For all k such that $0 \le k_{\min} \le k \le k_{\max} \le n$ solve the following LP model:

$$\max \sum_{i=1}^{n} c_i \cdot x_i$$
subject to:
$$\sum_{i=1}^{n} a_{ij} \cdot x_i \le b_j \qquad j = 1, \dots, m$$

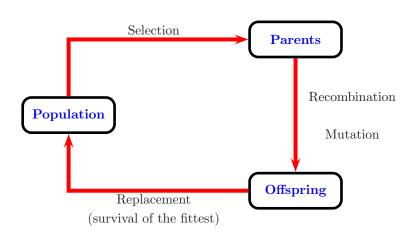
$$0 \le x_i \le 1 \qquad i = 1, \dots, n$$

$$\sum_{i=1}^{n} x_i = k$$

Main ideas of phase 2 of hybrid TS

- On the basis of the LP solutions from phase 1: produce integer solutions by rounding
- Use tabu search to search in the vicinity of these integer solutions
- Definition of vicinity: maximum allowed Hamming distance





KCT problem: a variation



Artificial Intelligence Research Institute (IIIA-CSIC)

Reference

C. Blum. **A new hybrid evolutionary algorithm for the** *k***-cardinality tree problem**, In: *Proceedings of GECCO 2006*, ACM Press, pages 515–522, 2006

KCT problem with node and edge weights

- **Given:** an undirected graph G = (V, E),
- Edge weights w_e , $\forall e \in E$, and node weights w_v , $\forall v \in V$
- A constant k < |V|
- **Optimization objective:** find a tree T_k in G with exactly k edges that minimizes

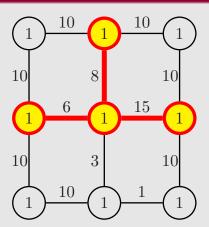
$$f(T_k) = \left(\sum_{e \in E(T_k)} w_e\right) + \left(\sum_{v \in V(T_k)} w_v\right)$$

KCT problem variant: example instance



Artificial Intelligence Research Institute (IIIA-CSIC)

Graphical illustration of an instance and a solution



KCT problem variant: dynamic programn

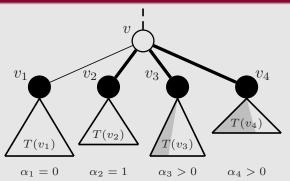


Artificial Intelligence Research Institute (IIIA-CSIC)

Observation

There exists a dynamic programming algorithm for solving the KCT problem in case G itself is a tree. **Complexity:** $\mathcal{O}(k^2|V|)$

Graphical illustration



Making use of DP within an EA



Artificial Intelligence Research Institute (IIIA-CSIC)

Note

This dynamic programming algorithm is used in the recombination/crossover operator

Case 1: parent solutions T_1 and T_2 share at least one node

- 1 Merge T_1 and $T_2 \rightarrow$ a graph G_c
- 2 Generate a minimum spanning tree (MST) T of G_c
- 3 Utilize DP for deriving the best tree with k edges in T

Case 2: parent solutions T_1 and T_2 do not share any node

- 1 Extend T_1 step by step using a greedy algorithm until it contects with $T_2 \to {\sf a}$ tree T that contains both T_1 and T_2
- 2 Utilize DP for deriving the best tree with k edges in T

Topics for the remainder of the course



Artificial Intelligence Research Institute (IIIA-CSIC)

Examples from our recent work

- **CMSA:** the algorithm *Construct, Merge, Solve & Adapt*
- ACO_neg: an ACO variant that makes use of negative learning
- Beam-ACO: an ACO variant that makes use of beam search

In our experience ...

LNS works especially well when the following two conditions are fulfilled:

- 1 The number of solution components is is not high
- 2 The number of components in a solution is not too small

Question

What kind of general algorithm can we apply when the above conditions are not fullfilled?

CMSA: main idea



Artificial Intelligence Research Institute (IIIA-CSIC)

Observation

In the presence of a large number of solutions components, many of them only lead to bad solutions

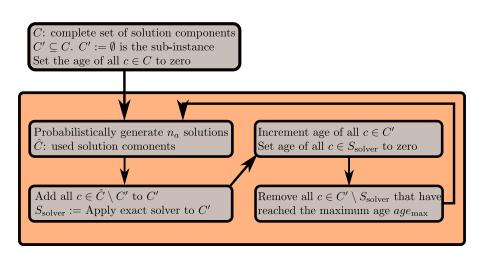
Idea

Exclude the presumably bad solution components from the ILP before solving it

Steps of one CMSA iteration

- Iteratively generate presumably good solutions in a probabilistic way
- Assemble a sub-instance from the used solution components
- Solve the sub-instance by means of an ILP solver
- Delete useless solution components from the sub-instance





Main diff. between CMSA and LNS



Artificial Intelligence Research Institute (IIIA-CSIC)

How is the original problem instance reduced? LNS **CMSA** Search Space Search Space Solutions that only contain Solutions that contain components from $C' \subseteq C$ partial solution S^p

- LNS: Partial destruction of the incumbent solution
- CMSA: Generating new solutions and removing old solution components

Application of CMSA: RFLCS problem



- The RFLCS problem is the LCS problem with an additional constraint: no letter may appear more than once in a valid solution
- Proposed in: 2010 in the journal Discrete Applied Mathematics
- Complexity: APX-hard (shown in the above article)
- Motivation: Genome rearrangement where duplicate genes are basically not considered
- Existing algorithms:
 - 1 Three simple heuristics, Discrete Applied Mathematics, 2010
 - 2 An evolutionary algorithm, *Operations Research Letters*, 2013

RFLCS problem: Best-Next heuristic



Artificial Intelligence Research Institute (IIIA-CSIC)

Best-Next: generates a solution from left to right

- 1: **input:** a problem instance (x, y, Σ)
- 2: **initialization:** $t := \epsilon$ (where ϵ is the empty string)
- 3: while $|\Sigma_t^{nd}| > 0$ do
- 4: $a := \mathsf{ChooseFrom}(\Sigma_t^{\mathsf{nd}})$
- 5: t := ta
- 6: end while
- 7: **output:** a repetition-free common subsequence *t*

Question

How is Σ_t^{nd} defined?



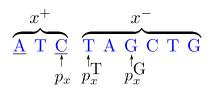
Artificial Intelligence Research Institute (IIIA-CSIC)

Example instance and partial solution

Given: $(x, y, \Sigma = \{A, C, T, G\})$ where

- $\mathbf{x} = \mathsf{ATCTAGCTG}$
- $\mathbf{v} = \mathsf{TACCATGTG}$

Partial solution: t = AC



$$\begin{array}{c}
y^{+} \\
 \hline
 T \underline{A} \underline{C} \\
 p_{y}
\end{array}$$

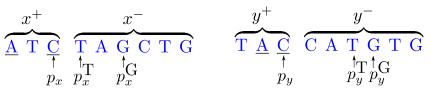
$$\begin{array}{c}
y^{-} \\
 C \underline{A} \underline{T} \underline{G} \underline{T} \underline{G} \\
 p_{y}^{\dagger} \underline{T} \underline{D} \underline{G} \\
 p_{y}^{\dagger} \underline{D} \underline{G} \\
 \end{array}$$

Therefore: $\Sigma_t^{nd} = \{T\}$



$$\eta(ta) := \left(\frac{p_x^a - p_x}{|x^-|} + \frac{p_y^a - p_y}{|y^-|}\right)^{-1}, \quad \forall a \in \Sigma_t^{\text{nd}}$$

$$\underbrace{\frac{x^{+}}{A} \quad T \quad C}_{p_{x}} \quad \underbrace{\frac{x^{-}}{f} \quad A \quad G \quad C \quad T \quad G}_{p_{x}}$$



RFLCS problem: ILP model

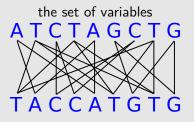


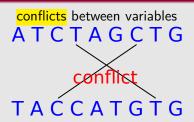
Artificial Intelligence Research Institute (IIIA-CSIC)

RFLCS problem: variables of the ILP model

The ILP model consists of a binary variable $z_{i,j}$ for each pair of positions $\frac{i}{\ln x}$ and $\frac{i}{j}$ in $\frac{y}{j}$ such that $\frac{x[i] = y[j]}{j}$.

Example







Artificial Intelligence Research Institute (IIIA-CSIC)

$$\max \sum_{z_{i:j} \in \mathcal{I}} z_{i,j} \tag{1}$$

subject to:

$$\sum_{z_{i,i} \in \mathcal{Z}_a} z_{i,j} \le 1 \quad \text{for } a \in \Sigma$$
 (2)

$$z_{i,j} + z_{k,l} \le 1$$
 for all $z_{i,j}$ and $z_{k,l}$ being in conflict (3)

$$z_{i,j} \in \{0,1\} \quad \text{for } z_{i,j} \in Z \tag{4}$$

Where ...

- $z_{i,j} \in Z_a$ if and only if x[i] = y[j] = a
- $z_{i,j}$ and $z_{k,l}$ are in conflict if and only if (i < k and j > l) or (i > k and j < l)

RFLCS problem: experiments



Artificial Intelligence Research Institute (IIIA-CSIC)

Set 1 of problem instances

30 instances for each combination of ...

- Length of the input strings: $n \in \{32, 64, 128, 256, 512, 1024, 2048, 4096\}$
- Alphabet size: $|\Sigma| \in \{n/8, n/4, 3n/8, n/2, 5n/8, 3n/4, 7n/8\}$

Set 2 of problem instances

30 instances for each combination of ...

- Alphabet size: $|\Sigma| \in \{4, 8, 16, 32, 64, 128, 256, 512\}$
- Maximal number of repetitions of each letter: $rep \in \{3, 4, 5, 6, 7, 8\}$

Parameter tuning: CMSA

The parameters of CMSA are tuned by irace for each alphabet size.

RFLCS problem: **CPLEX** performance



Artificial Intelligence Research Institute (IIIA-CSIC)

Set 1

- Length of the input strings: $n \in \{32, 64, 128, 256, 512, 1024, 2028, 4048\}$
- Alphabet size: $|\Sigma| \in \{n/8, n/4, 3n/8, n/2, 5n/8, 3n/4, 7n/8\}$

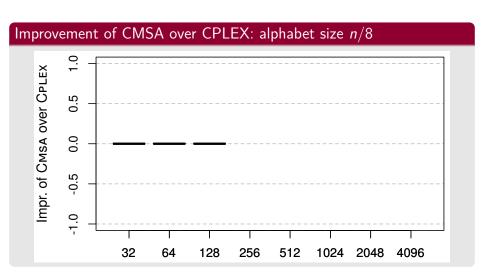
Set 2

- Alphabet size: $|\Sigma| \in \{4, 8, 16, 32, 64, 128, 256, 512\}$
- Maximal number of repetitions of each letter: $rep \in \{3, 4, 5, 6, 7, 8\}$

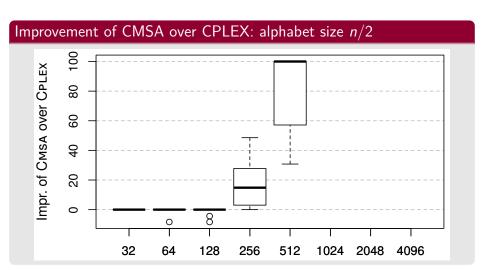
Summary

CPLEX is able to solve nearly all existing problem instances from the literature to optimality

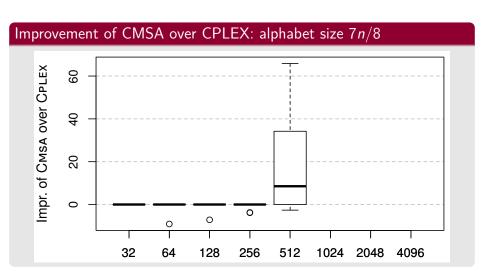




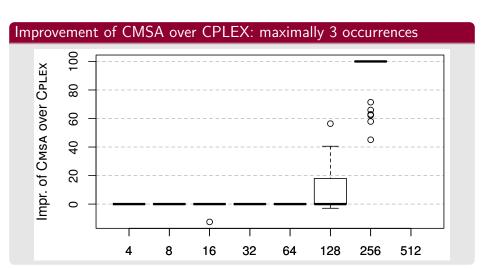




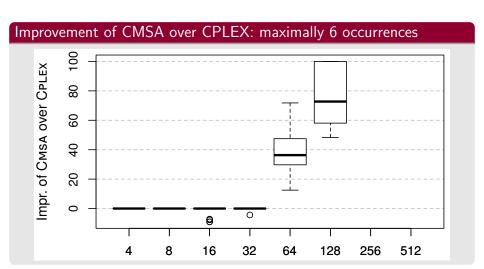




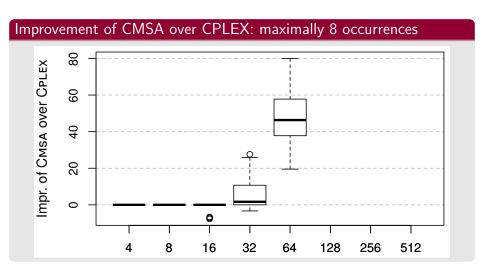






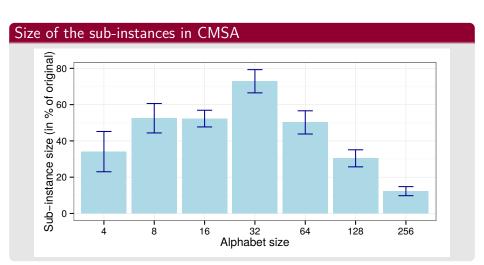






CMSA: size of sub-instances





CMSA application 2: MCSP problem



Artificial Intelligence Research Institute (IIIA-CSIC)

Minimum common string partition (MCSP) problem

- **Given:** Two **related sequences** of length n over alphabet Σ
- 2 **Note:** Sequences s_1 and s_2 are called related if and only if each letter appears the same number of times in each sequence

Valid solutions

- Generate a partition P_1 of sub-sequences of s_1 without overlap
- Generate a partition P_2 of sub-sequences of s_2 without overlap
- Solution $S = (P_1, P_2)$ is valid if and only if $P_1 = P_2$
- **Objective function:** $f(S) := |P_1| = |P_2|$
- Optimization objective: minimization

Additional information

- Introduced in 2005 in the context of genome rearrangement
- Complexity: NP-hard



Artificial Intelligence Research Institute (IIIA-CSIC)

Example instance and solutions

- $s_1 := AGACTG$, $s_2 := ACTAGG$
- Trivial solution:
 - $P_1 = P_2 = \{A, A, C, T, G, G\}$
 - Objective function value: 6
- Optimal solution S^* :
 - $P_1 = P_2 = \{ACT, AG, G\}$
 - **Objective function value:** 3

Algorithmic solutions from the literature

- 2005: a greedy heuristic
- 2007: an approximation algorithm
- 2008: a fixed-parameter tractability (FPT) study
- 2013: ant colony optimization metaheuristic

Model of the MCSP problem



Artificial Intelligence Research Institute (IIIA-CSIC)

Definition: given s_1 and s_2 ...

- A common block b_i is a triplet $(t_i, k1_i, k2_i)$ where t_i is a sequence ...
 - 1 starting at position $1 \le k1_i \le n$ in s_1
 - 2 starting at position $1 \le k2_i \le n$ in s_2
- B is the set of all common blocks of s_1 and s_2
- \blacksquare Any (partial) solution S is a subset of B such that
 - 1 $\sum_{b_i \in S} |t_i| = n$ (in case of a **complete solution**)
 - 2 $\sum_{b_i \in S} |t_i| < n$ (in case of a partial solution)
 - 3 For every pair $b_i, b_j \in S$: t_i and t_j do not overlap neither in s_1 nor in s_2

Example for this MCSP model



Artificial Intelligence Research Institute (IIIA-CSIC)

Input sequences

$$s_1 = AGACTG$$
 and $s_2 = ACTAGG$

Set B of all common blocks

$$\begin{cases} b_1 = (\mathsf{ACT}, \ 3, \ 1) & b_8 = (\mathsf{A}, \ 3, \ 4) \\ b_2 = (\mathsf{AG}, \ 1, \ 4) & b_9 = (\mathsf{C}, \ 4, \ 2) \\ b_3 = (\mathsf{AC}, \ 3, \ 1) & b_{10} = (\mathsf{T}, \ 5, \ 3) \\ b_4 = (\mathsf{CT}, \ 4, \ 2) & b_{11} = (\mathsf{G}, \ 2, \ 5) \\ b_5 = (\mathsf{A}, \ 1, \ 1) & b_{12} = (\mathsf{G}, \ 2, \ 6) \\ b_6 = (\mathsf{A}, \ 1, \ 4) & b_{13} = (\mathsf{G}, \ 6, \ 5) \\ b_7 = (\mathsf{A}, \ 3, \ 1) & b_{14} = (\mathsf{G}, \ 6, \ 6) \end{cases}$$

Solution and set of solution components

- Solution $\{ACT, AG, G\}$ corresponds to $S = \{b_1, b_2, b_{14}\}$
- **Note:** The set *B* is the set of all solution components

MCSP problem: ILP model (1)



Artificial Intelligence Research Institute (IIIA-CSIC)

Input sequences

 $s_1 = AGACTG$ and $s_2 = ACTAGG$

$$B = \begin{cases} b_1 = (\mathsf{ACT}, \ 3, \ 1) \\ b_2 = (\mathsf{AG}, \ 1, \ 4) \\ b_3 = (\mathsf{AC}, \ 3, \ 1) \\ b_4 = (\mathsf{CT}, \ 4, \ 2) \\ b_5 = (\mathsf{A}, \ 1, \ 1) \\ b_6 = (\mathsf{A}, \ 1, \ 4) \\ b_7 = (\mathsf{A}, \ 3, \ 1) \\ b_8 = (\mathsf{A}, \ 3, \ 4) \\ b_9 = (\mathsf{C}, \ 4, \ 2) \\ b_{10} = (\mathsf{T}, \ 5, \ 3) \\ b_{11} = (\mathsf{G}, \ 2, \ 5) \\ b_{12} = (\mathsf{G}, \ 2, \ 6) \\ b_{13} = (\mathsf{G}, \ 6, \ 5) \\ b_{14} = (\mathsf{G}, \ 6, \ 6) \end{cases}$$

$$B = \begin{cases} b_1 = (\mathsf{ACT}, \ 3, \ 1) \\ b_2 = (\mathsf{AG}, \ 1, \ 4) \\ b_3 = (\mathsf{AC}, \ 3, \ 1) \\ b_4 = (\mathsf{CT}, \ 4, \ 2) \\ b_5 = (\mathsf{A}, \ 1, \ 1) \\ b_6 = (\mathsf{A}, \ 1, \ 4) \\ b_7 = (\mathsf{A}, \ 3, \ 1) \\ b_8 = (\mathsf{A}, \ 3, \ 4) \\ b_9 = (\mathsf{C}, \ 4, \ 2) \\ b_{10} = (\mathsf{T}, \ 5, \ 3) \\ b_{11} = (\mathsf{G}, \ 2, \ 5) \\ b_{12} = (\mathsf{G}, \ 2, \ 6) \\ b_{13} = (\mathsf{G}, \ 6, \ 6) \end{cases}$$

$$M1 = \begin{cases} 0 & 0 & 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{cases}$$

$$M2 = \begin{pmatrix} 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$



Artificial Intelligence Research Institute (IIIA-CSIC)

ILP model: MCSP problem

$$\min \sum_{i=1}^m x_i$$

subject to:

$$\sum_{i=1}^{m} |t_i| \cdot x_i = n$$

$$\sum_{i=1}^{m} M1_{i,j} \cdot x_i = 1 \text{ for } j = 1, \dots, n$$

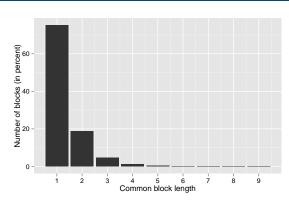
$$\sum_{i=1}^{m} M2_{i,j} \cdot x_i = 1 \text{ for } j = 1, \dots, n$$

$$x_i \in \{0, 1\} \text{ for } i = 1, \dots, m$$

MCSP problem: set of common blocks



Artificial Intelligence Research Institute (IIIA-CSIC)



Note

- An instance consists of many solution components
- The vast majority of common blocks of length 1 and 2 will not form part of good solutions

MCSP problem: greedy heuristic



Artificial Intelligence Research Institute (IIIA-CSIC)

Simple greedy heuristic

- \blacksquare At each construction step we add exactly one common block to the partical solution $S_{\rm parcial}$
- Given a partial solution S_{parcial} , $N(S_{\text{parcial}}) \subset B$ denotes the set of common blocks that can be added to S_{parcial}

Pseudo code

- 1 $S_{\text{parcial}} := \emptyset$
- **2** while $S_{
 m parcial}$ is not a complete solution
 - Select a largest common block b_i from $N(S_{parcial})$
 - lacksquare $S_{
 m parcial} := S_{
 m parcial} \cup \{b_i\}$

Note

This greedy heuristic is used in a probabilistic way within CMSA

Problem instances and tuning



Artificial Intelligence Research Institute (IIIA-CSIC)

Problem instances

- In total: 300 instances
- Input sequence length: $n \in \{200, 400, \dots, 1800, 2000\}$
- Alphabet size: $|\Sigma| \in \{4, 12, 20\}$

Parameter tuning with irace

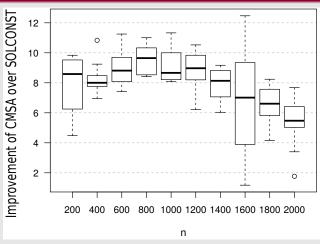
n	na	age _{max}	$d_{ m rate}$	$I_{ m size}$	t _{max}
400	50	10	0.0	10	60
800	50	10	0.5	10	240
1200	50	10	0.9	10	480
1600	50	5	0.9	10	480
2000	50	10	0.9	10	480

Performance of CMSA (1)



Artificial Intelligence Research Institute (IIIA-CSIC)

Improvement of CMSA over the greedy heuristic: $|\Sigma|=4$

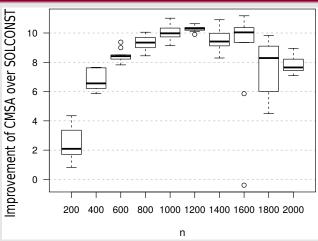


Performance of CMSA (2)



Artificial Intelligence Research Institute (IIIA-CSIC)

Improvement of CMSA over the greedy heuristic: $|\Sigma|=12$

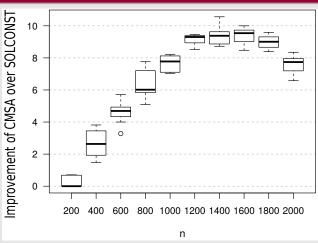


Performance of CMSA (3)



Artificial Intelligence Research Institute (IIIA-CSIC)

Improvement of CMSA over the greedy heuristic: $|\Sigma| = 20$

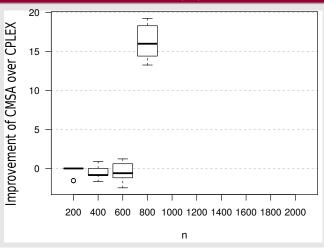


Performance of CMSA (4)



Artificial Intelligence Research Institute (IIIA-CSIC)

Improvement of CMSA over CPLEX: $|\Sigma| = 4$

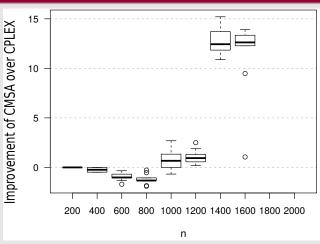


Performance of CMSA (5)



Artificial Intelligence Research Institute (IIIA-CSIC)

Improvement of CMSA over CPLEX: $|\Sigma|=12$

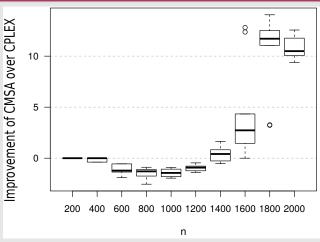


Performance of CMSA (6)



Artificial Intelligence Research Institute (IIIA-CSIC)

Improvement of CMSA over CPLEX: $|\Sigma| = 20$



Questions?





Extending ACO with negative learning



- **Observation:** ACO is based on learning from positive examples
- **Nature shows:** learning from negative examples can be useful



IIIA PhD Student Teddy Nurcahyadi



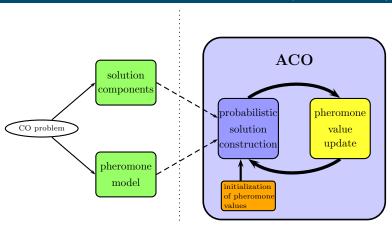
ANTS 2020

Best Paper Award

Extending ACO with negative learning



Artificial Intelligence Research Institute (IIIA-CSIC)



Note

- ACO has been applied to many combinatorial optimization problems
- The type of learning used is positive learning

Negative learning in nature



Artificial Intelligence Research Institute (IIIA-CSIC)

Observation

Behavior of certain insects is governed not only by reward, but also by penalty / punishment

Examples

- Pharaoh Ant (Monomorium pharaonis) → mark routes leading to non-profitable food source [Robinson 2005, 2007]
- Honey Bees (Apis mellifera linguistica) \rightarrow mark flowers that are already exhausted of nectar [Giurfa 1993]
- Black garden-ants (Lasius niger) \rightarrow enables the colony to maintain a flexible foraging system [Grueter 2012]
- Tsetse flies (Glossina morsitans) and house flies (Musca domestica)

 → prevents wasteful activities related to their reproduction behaviour
 [Schlein 1981]

Previous attempts



Artificial Intelligence Research Institute (IIIA-CSIC)

Negative learning approaches from the literature

- [Maniezzo 1999] and [Cordón et al. 2000] were the first ones to make use of an active decrease of pheromone values associated to solution components appearing in low-quality solutions.
- **Montgommery et al. 2002**] proposed the first strategy using explicitly anti-pheromone values.
- Ramos 2013] proposed a method that uses a coevolved compromise between positive and negative feedback.
- **Simons et al. 2016]** explored different extensions of the approaches from [Montgommery et al. 2002].
- **Rojas et al. 2018**] proposed a mechanism based on opposite learning.

However

None of these approaches is much used nowadays.



Application to the MDS problem



Artificial Intelligence Research Institute (IIIA-CSIC)

Baseline algorithm: MMAS

■ Negative learning mechanisms is implemented on top of a standard ACO algorithm: \mathcal{MAX} - \mathcal{MIN} Ant System (MMAS) in the hypercube framework (Blum, Dorigo, 2004).

Main Characteristics of the Baseline Algorithm

- At each iteration: n_a solutions are probabilistically generated both based on pheromone and on greedy information
- 2 The pheromone values are modified using (at most) three solutions: the best-so-far, the iteration-best and the restart-best solutions
- 3 Restarts are performed once convergence is detected



Artificial Intelligence Research Institute (IIIA-CSIC)

Pheromone models

- **Standard pheromones:** A pheromone value τ_i for each vertex v_i of the input graph
- Negative pheromones: A pheromone value τ_i^{neg} for each vertex v_i

Solution construction probabilities

Given a partial solution S

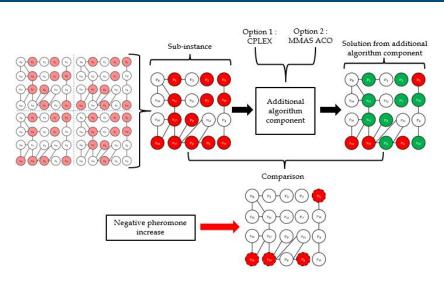
$$\mathbf{p}(v_k \mid S) := \frac{\eta_k \cdot \tau_k \cdot (1 - \tau_k^{\text{neg}})}{\sum_{v_l \in V \setminus S} \eta_l \cdot \tau_l \cdot (1 - \tau_l^{\text{neg}})}$$

Note

 $\mathbf{p}(v_k \mid S)$ is the probability to chose v_k as the next vertex to be added to S

ACO + negative learning: main idea





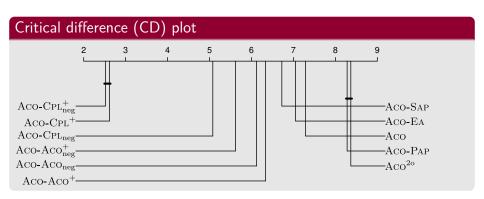


- Baseline algorithm:
 - Aco
- Our negative learning variants:
 - \blacksquare $\mathrm{Aco\text{-}CPL}_{\mathrm{neg}}^+ :$ negative learning + using CPLEX result for positive learning
 - \blacksquare $A{\rm CO\text{-}CPL}_{neg}{:}$ negative learning
 - ACO-CPL⁺: only using CPLEX result for positive learning
 - \blacksquare Aco-Aco $_{\text{neg}}^+$
 - Aco-Aco_{neg}
 - Aco-Aco⁺
- 3 Negative learning variants from the literature:
 - Aco-Sap, Aco-Pap, Aco-Ea, Aco²⁰

Global results for 160 MDS instances



Artificial Intelligence Research Institute (IIIA-CSIC)



Observations

- Our variants outperform the baseline Aco and the other competitors
- The Aco-CPL variants perform better than the Aco-Aco variants

Comparison to the state-of-the-art



Artificial Intelligence Research Institute (IIIA-CSIC)

Comparison

Instance family	CC^2FS	FastMWDS	RLS_o	ScBppw	FastDS	Aco-Cpl ⁺ _{neg}
V50U150	12.9	12.9	12.9	12.9	12.9	12.9
V50U200	9.4	9.4	9.4	9.4	9.4	9.4
V100U150	17.0	17.0	17.0	17.3	17.0	17.0
V100U200	10.4	10.4	10.4	10.6	10.4	10.4
V250U150	18.0	18.0	18.0	19.0	18.0	18.0
V250U200	10.8	10.8	10.8	11.5	10.8	10.8
V500U150	18.5	18.5	18.6	20.1	18.5	18.5
V500U200	11.2	11.2	11.2	12.4	11.2	11.2
V800U150	19.0	19.0	19.1	20.9	19.0	19.0
V800U200	11.7	11.7	11.9	12.6	11.8	11.7
V1000U150	19.1	19.1	19.2	21.3	19.1	19.1
V1000U200	12.0	12.0	12.0	13.0	12.0	12.0

Competitors

- CC²FS ([Wang, Cai, and Yin, 2017])
- FastMWDS ([Wang, Cai, Chen et al., 2018])
- RLS_o ([Chalupa, 2018])
- ScBppw ([Fan et al., 2019])
- FastDS ([Cai et al., 2020])

Questions?





Hybridization example: Beam-ACO



Artificial Intelligence Research Institute (IIIA-CSIC)

What is Beam-ACO?

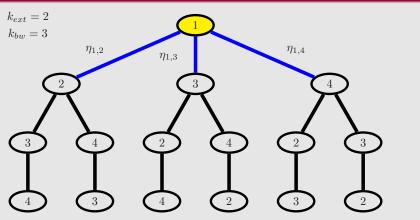
- Beam-ACO is a hybrid algorithm that results from the combination of ant colony optimization with a tree search method called beam search.
- Main publication: Blum, C. (2005). Beam-ACO, Hybridizing ant colony optimization with beam search: An application to open shop scheduling. Computers & Operations Research, 32(6), 1565-1591.

Beam search for the TSP (1)



Artificial Intelligence Research Institute (IIIA-CSIC)

First construction step

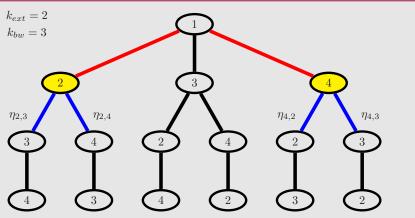


Beam search for the TSP (2)



Artificial Intelligence Research Institute (IIIA-CSIC)

Second construction step

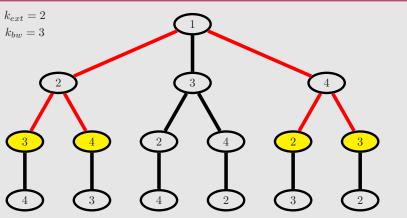


Beam search for the TSP (3)



Artificial Intelligence Research Institute (IIIA-CSIC)

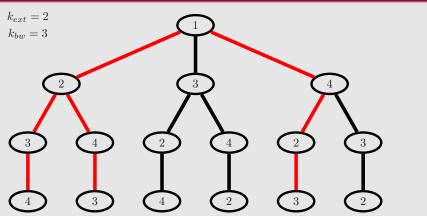
After the 2nd construction step: use of a lower bound





Artificial Intelligence Research Institute (IIIA-CSIC)

Third construction step



Beam-ACO: basic idea



Artificial Intelligence Research Institute (IIIA-CSIC)

Basic idea of Beam-ACO

- Instead of n_a independent solution constructions per iteration: perform a probabilistic beam search with beam width $k_{bw} = n_a$.
- The probabilities for the construction steps are calculated on the basis of (1) the greedy function and (2) the pheromone values, just like in ACO.

Advantages of Beam-ACO

- Strong heuristic guidance by a lower bound
- Embedded in the adaptive ACO framework
- Beam-ACO utilizes two types of complementary problem knowledge (heuristic + lower bound)

Beam-ACO: applications



Artificial Intelligence Research Institute (IIIA-CSIC)

Applications of Beam-ACO (a selection)

- Open shop scheduling (OSS)
 Blum, Computers & Operations Research (2005)
- Supply chain management
 Caldeira et al., FUZZ-IEEE 2007, ISFA 2007
- Simple assembly line balancing (SALB)
 Blum, INFORMS Journal on Computing (2008)
- Travelling salesman problem with time windows (TSPTW)
 López-Ibañez et al., Computers & Operations Research (2010)
- Longest common subsequence (LCS) problems
 Blum et al. CEC 2010, EA 2013, Journal of Heuristics (2016)
- Weighted vehicle routing problem
 Tang et al. IEEE Transactions on Automation Science and Engineering (2014)

Questions?



