Combining Metaheuristics based on Solution Construction with Exact Techniques

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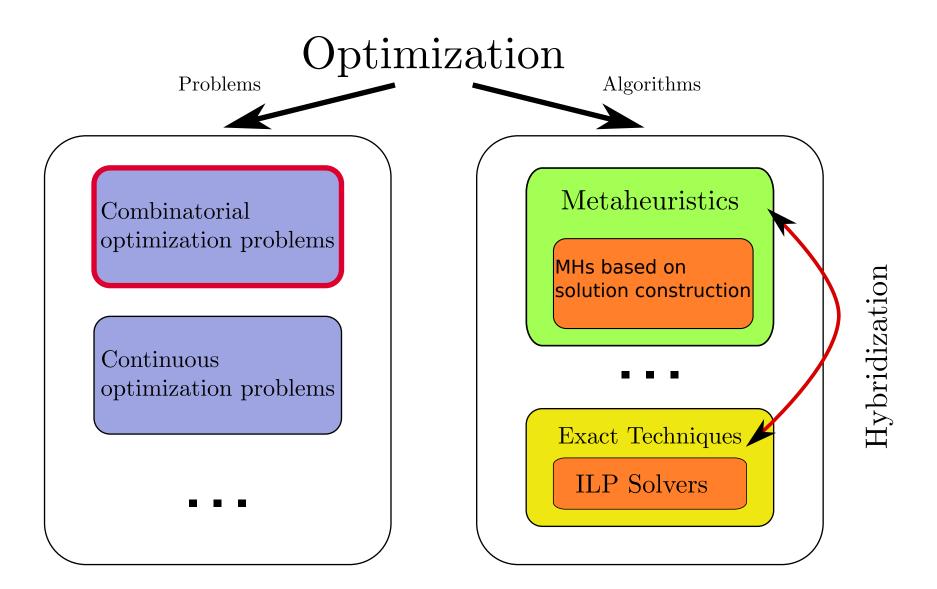


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Preliminaries: Preparing the Grounds



Outline

- **Hybrid Metaheuristics**
- ► **Approach 1: Beam-ACO** (2005)
- ► Approach 2: Construct, Merge, Solve & Adapt (CMSA) (2015)
- ► **Application:** Repetition-free Longest Common Subsequence
- **Relation:** CMSA with Large Neighborhood Search
- Conclusions / Future Work

Hybrid metaheuristics: definition

Definition: What is a hybrid metaheuristic?

Problem: a precise definition is not possible/desirable

Possible characterization:

A technique that results from the combination of a metaheuristic with other techniques for optimization

What is meant by: other techniques for optimisation?

- Metaheuristics
- Branch & bound
- Dynamic programming
- ▶ Integer Linear Programming (ILP) techniques

Hybrid metaheuristics: history

History:

- ► For a long time the different communities co-existed quite isolated
- ▶ Hybrid approaches were developed already early, but only sporadically
- Only since about 15 years the published body of research grows significantly:
 - 1. 1999: CP-AI-OR Conferences/Workshops
 - 2. 2004: Workshop series on Hybrid Metaheuristics (HM 200X)
 - **3. 2006:** Matheuristics Workshops

Consequence: The term hybrid metaheuristics identifies a new line of research

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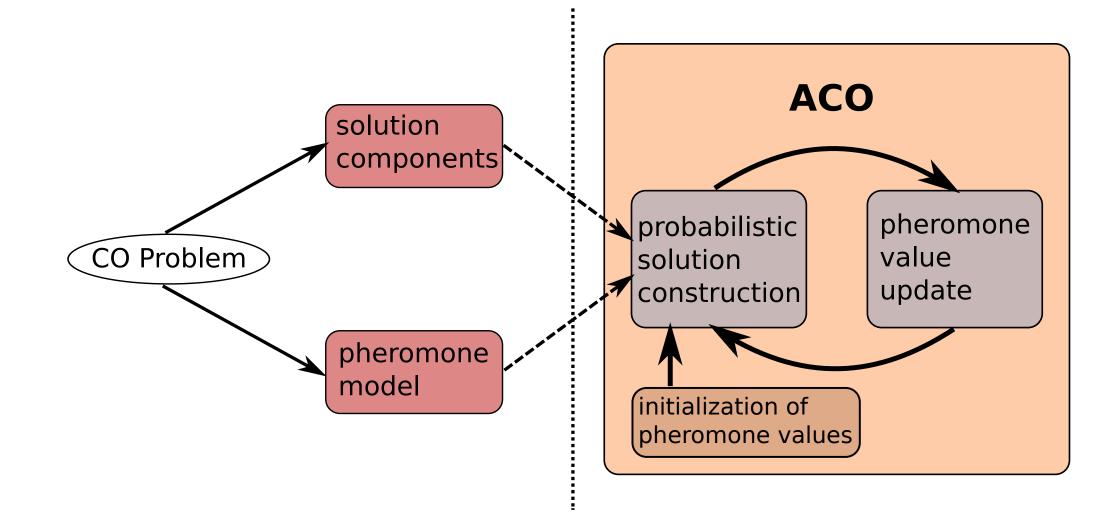
Motivation behind my work on hybrid metaheuristics

- ▶ In the field of metaheuristics we have rules of thumb :
 - 1. If, for your problem, there is a **good greedy heuristic** apply **GRASP** or Iterated Greedy
 - 2. If, for your problem, there is an **efficient neighborhood** apply Iterated Local Search or Tabu Search
- ▶ In contrast, for hybrid metaheuristics not much is known
 - * We only have very few generally applicable techniques
 - \star We do not really know for which type of problem they work well

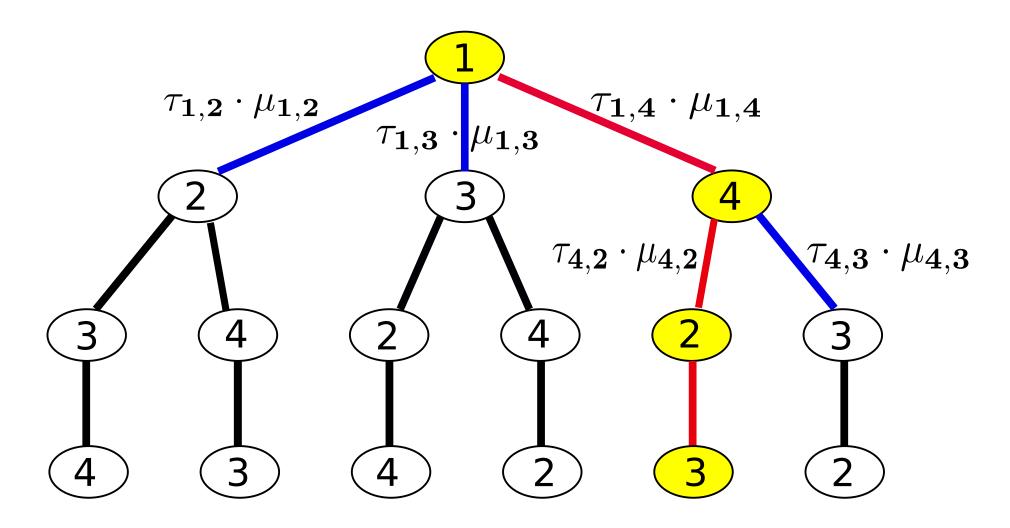
Beam-ACO

Short description

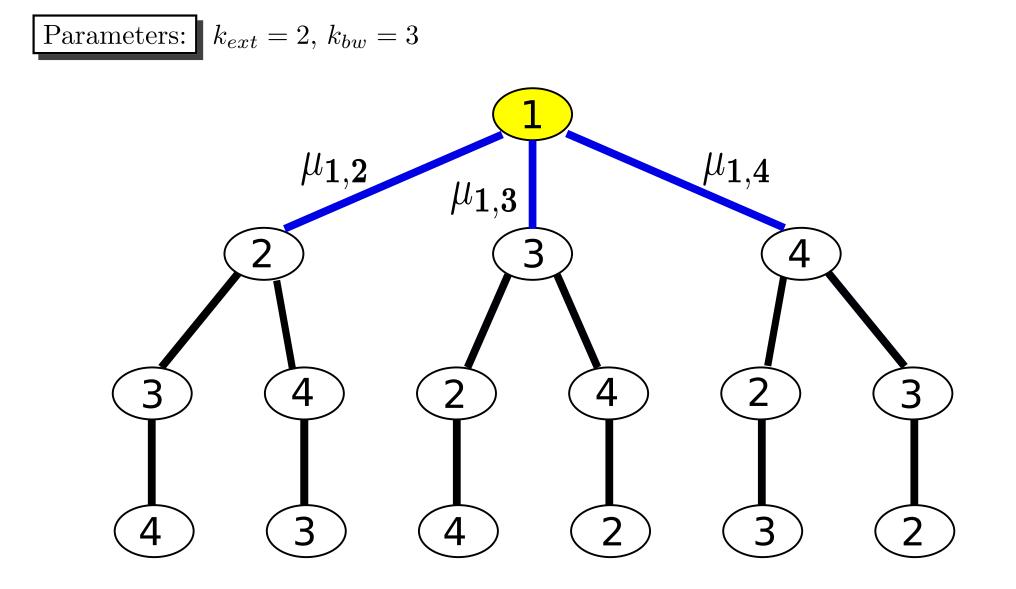
Ant Colony Optimization (ACO)



ACO is a tree search algorithm

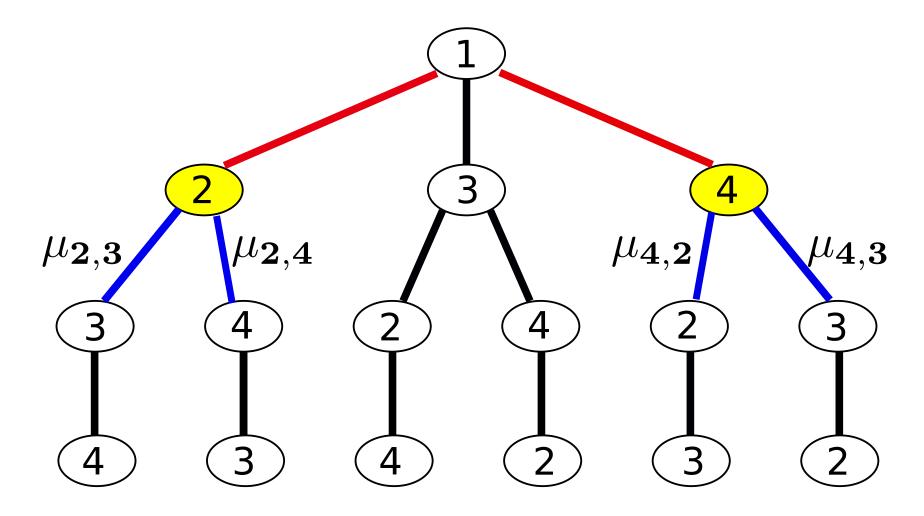


Beam search: 1st construction step



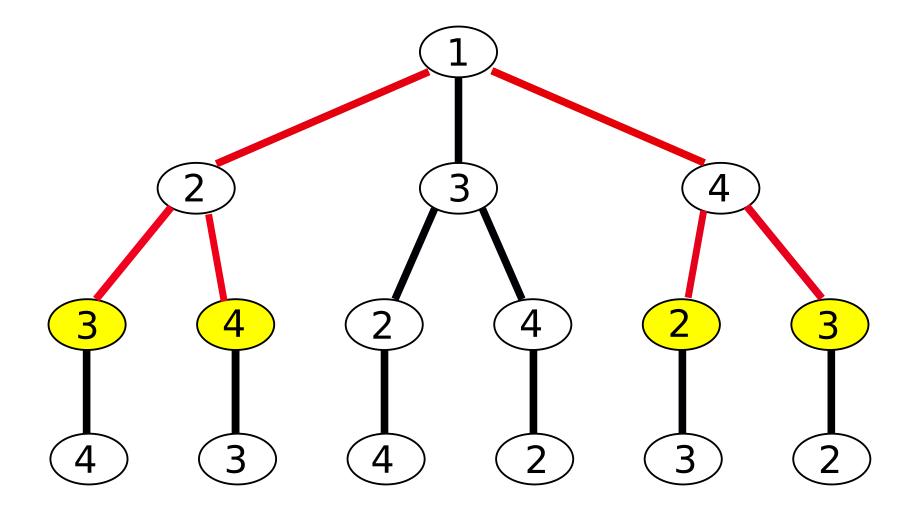
Beam search: 2nd construction step

Parameters: $k_{ext} = 2, k_{bw} = 3$



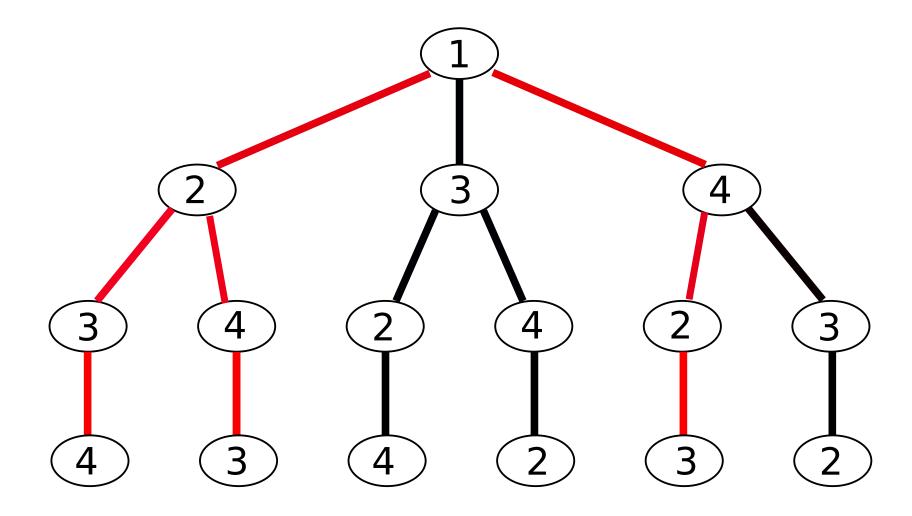
Beam search: after 2nd construction step

Use of: lower (upper) bound



Beam search: 3rd construction step

Parameters: $k_{ext} = 2, k_{bw} = 3$



Hybrid algorithm: Beam-ACO

Idea:

Instead of n_a independent solution constructions per iteration,

▶ perform a probabilistic beam search with beam width $k_{bw} = n_a$

Advantages:

- Strong heuristic guidance by a lower bound
- > Embedded in the adaptive framework of ACO

Requirements for the lower bound:

▶ Fast to compute

▶ Differentiate well between nodes on the same level of the search tree

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Hybrid algorithm: Beam-ACO

Applications Beam-ACO was applied to the following problems:

- ▶ 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)

Hybrid algorithm: Beam-ACO

Question: Why does it work so well?

Observation: Beam-ACO uses 2 types of complementary problem information

- 1. A greedy function
- 2. Lower (respectively, upper) information

These two types of information are especially well exploited in Beam-ACO!

Construct, Merge, Solve & Adapt (CMSA)

Short description

Why combining metaheuristics with ILP Solvers?

General advantage of metaheuristics:

- ► Very good in exploiting information on the problem (greedy heuristics)
- Generally very good in obtaining high-quality solutions for medium and even large size problem instances

However:

- ▶ Metaheuristics may also reach their limits with growing problem instance size
- ▶ Metaheuristics fail when the information on the problem is misleading

Goal: Taking profit from valuable optimization expertise that went into the development of ILP solvers even in the context of large problem instances

Standard: Large Neighborhood 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 neighborhoods:

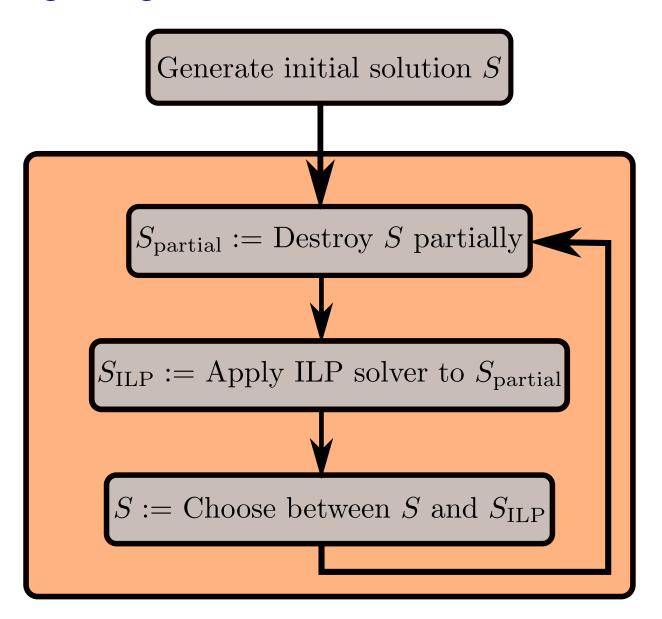
- 1. Advantage: The average quality of the local minima is high
- 2. **Disadvantage:** Finding an improving neighbor might itself be *NP*-hard due to the size of the neighborhood

Ways of examining large neighborhoods:

> Heuristically

Exact techniques: for example an ILP solver

ILP-based large neighborhood search: ILP-LNS



Hypothesis and resulting research question

In our experience: LNS works especially well when

- 1. The number of solution components (variables) is is not high
- 2. The number of components in a solution is not too small



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

Construct, Merge, Solve & Adapt: Principal Idea

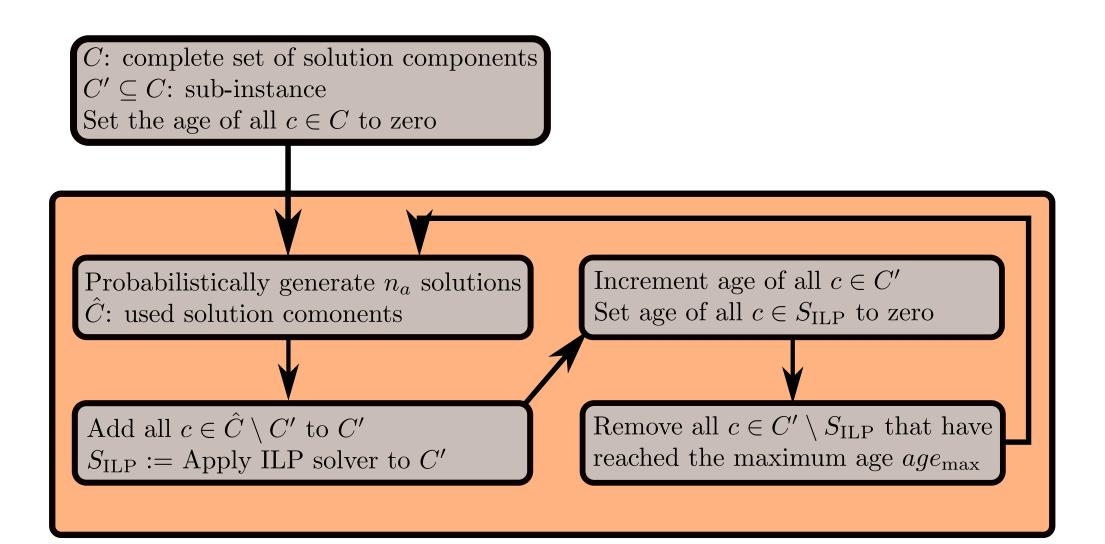
Observation: In the presence of a large number of solutions components, many of them only lead to bad solutions

Idea: Exclude the presumably bad solution components from the ILP

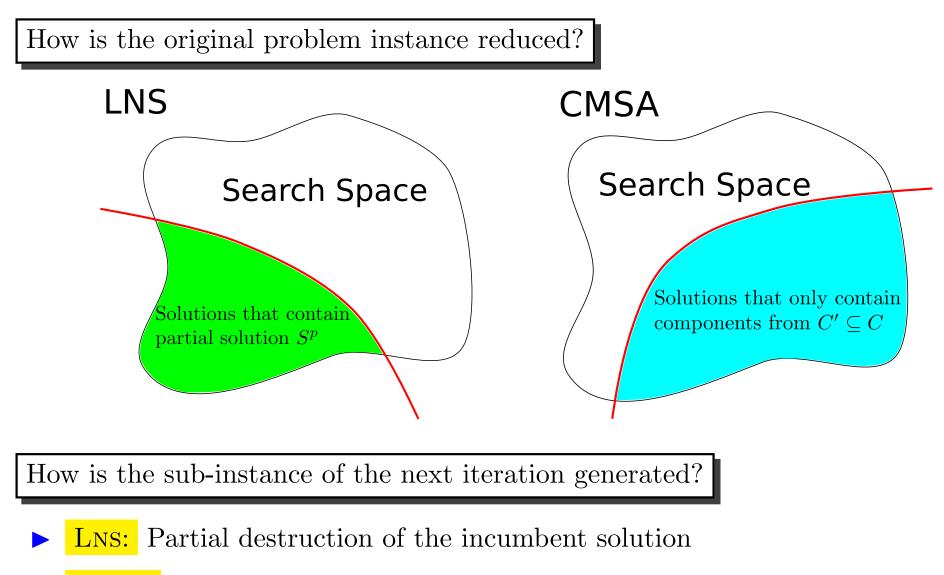
Steps of the proposed method:

- 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

Construct, Merge, Solve & Adapt: Flow Diagram



Differences between ${\rm LNS}$ and ${\rm CMSA}$: summarized



CMSA: Generating new solutions and removing **old** solution components

Longest common subsequence (LCS) problem (1)

Notation: What is a subsequence of a string?

A string t is called a subsequence of a string x,

iff t can be produced from x by deleting characters

Example: Is AAT a subsequence of ACAGTTA?

ACAGTTA

Longest common subsequence (LCS) problem (2)

Problem definition (restricted to two input sequence)

Give	
	n•
	L T •

A problem instance (x, y, Σ) , where

 \triangleright x and y are input sequences over the alphabet Σ

Optimization goal:

Find a longest string t^* that is a subsequence of strings x and $y \rightarrow$ a longest common subsequence

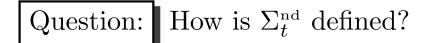
Repetition-free longest common subsequence problem

- **Restriction:** No letter **may appear more than once** in a valid solution
- Proposed in: 2010 in Discrete Applied Mathematics
- ► Hardness: APX-hard (shown in above paper)
- 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

A simple constructive RFLCS heuristic: Best-Next (1)

Principle: Builds a solution sequentially from left to right

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

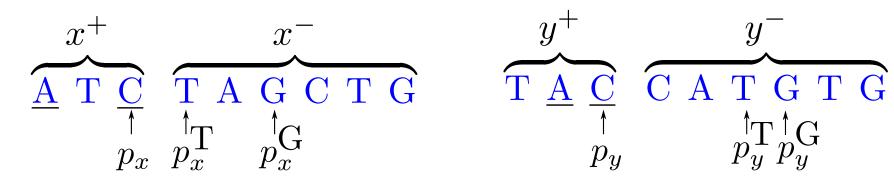


A simple constructive LCS heuristic: Best-Next (2)

Example: Given is

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

- $\star \ x = \text{ATCTAGCTG}$
- $\star y = \text{TACCATGTG}$
- $\blacktriangleright \quad \text{Partial solution} \quad t = \text{AC}$



Result: $\Sigma_t^{nd} = \{\mathbf{T}\}$

Greedy function

Greedy function:

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

$$\underbrace{\underbrace{A} T \underbrace{C}_{\uparrow} \underbrace{T}_{p_{x}} \underbrace{C}_{p_{x}} \underbrace{T}_{p_{x}} \underbrace{A} \underbrace{G}_{p_{x}} \underbrace{C}_{q_{x}} \underbrace{T}_{p_{x}} \underbrace{G}_{p_{x}} \underbrace{C}_{q_{x}} \underbrace{T}_{p_{x}} \underbrace{G}_{p_{x}} \underbrace{T}_{p_{x}} \underbrace{G}_{p_{x}} \underbrace{T}_{p_{x}} \underbrace{G}_{p_{y}} \underbrace{G}_{p_{y}} \underbrace{T}_{p_{y}} \underbrace{G}_{p_{y}} \underbrace{G}_{$$

Pheromone model

τ_{x,i}: desirability to add the letter at position i of string x to the solution
 τ_{y,i}: desirability to add the letter at position i of string y to the solution

Transition probabilities in Beam-ACO: given partial solution t,

$$\mathbf{p}(ta) = \frac{\left(\min\{\tau_{x,p_x^a}, \tau_{y,p_y^a}\} \cdot greedyinfo\right)}{\sum_{b \in \Sigma_t^{nd}} \left(\min\{\tau_{x,p_x^b}, \tau_{y,p_y^b}\} \cdot greedyinfo\right)} \quad , \forall \ a \in \Sigma_t^{nd}$$

Upper bound function

Given a partial solution t:

- \blacktriangleright Each input string x is partitioned into
 - 1. $x^+ :=$ first part of x until p_x
 - 2. $x^- :=$ remaining part of x (after p_x)

▶ $\delta(a, x)$ evaluates to 1 if letter a appears at least once in x^- , to 0 otherwise.

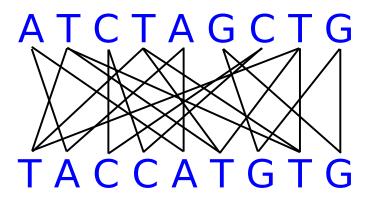
$$UB(t) := |t| + \sum_{a \in \Sigma_t} \min\{\delta(a, x), \delta(a, y)\}$$

ILP Model (1)

Set of binary variables:

For each position i of x and j of y such that x[i] = y[j] the model has a variable $z_{i,j}$

Example set of variables



Example of a conflict A T C T A G C T G conflict T A C C A T G T G

ILP Model (2)

$$\max \sum_{z_{i,j} \in Z} z_{i,j}$$
(1)
subject to:

$$\sum_{z_{i,j} \in Z_a} z_{i,j} \le 1 \text{ for } a \in \Sigma$$
(2)

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

$$z_{i,j} \in \{0,1\} \text{ for } z_{i,j} \in Z$$
(4)

Hereby:

►
$$z_{i,j} \in Z_a$$
 iff $x[i] = y[j] = a$

▶ $z_{i,j}$ and $z_{k,l}$ are in conflict iff i < k and j > l OR i > k and j < l

Experimental evaluation: benchmark instances

Set1: 30 instances for each combination of

- Input sequence length: $n \in \{32, 64, 128, 256, 512, 1024, 2028, 4048\}$
- Alphabet size: $|\Sigma| \in \{n/8, n/4, 3n/8, n/2, 5n/8, 3n/4, 7n/8\}$

Set2: 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: $rep \in \{3, 4, 5, 6, 7, 8\}$

Tuning: CMSA's and BEAM-ACO's parameters are tuned by irace for each alphabet size

Experimental results: performance of CPLEX

Set1:

- ▶ Input sequence length: $n \in \{32, 64, 128, 256, 512, 1024, 2028, 4048\}$
- ► Alphabet size: $|\Sigma| \in \{n/8, n/4, 3n/8, n/2, 5n/8, 3n/4, 7n/8\}$

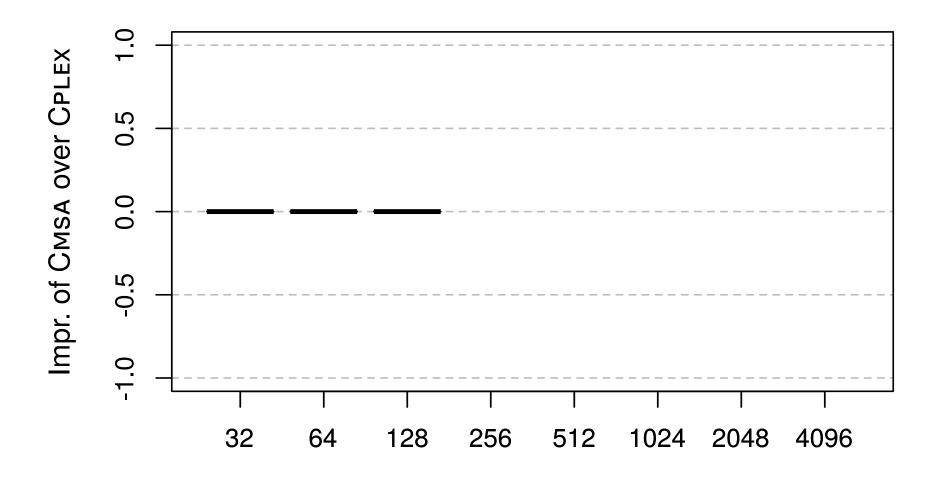
Set2:

• Alphabet size: $|\Sigma| \in \{4, 8, 16, 32, 64, 128, 256, 512\}$

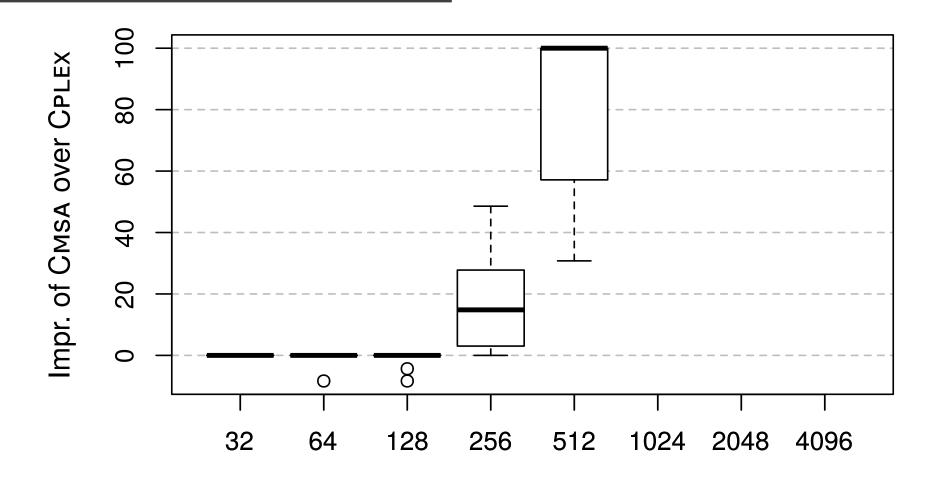
Maximal number of repetitions of each letter: $rep \in \{3, 4, 5, 6, 7, 8\}$

Result: CPLEX is able to solve nearly all exisiting problem instances from the literature to optimality

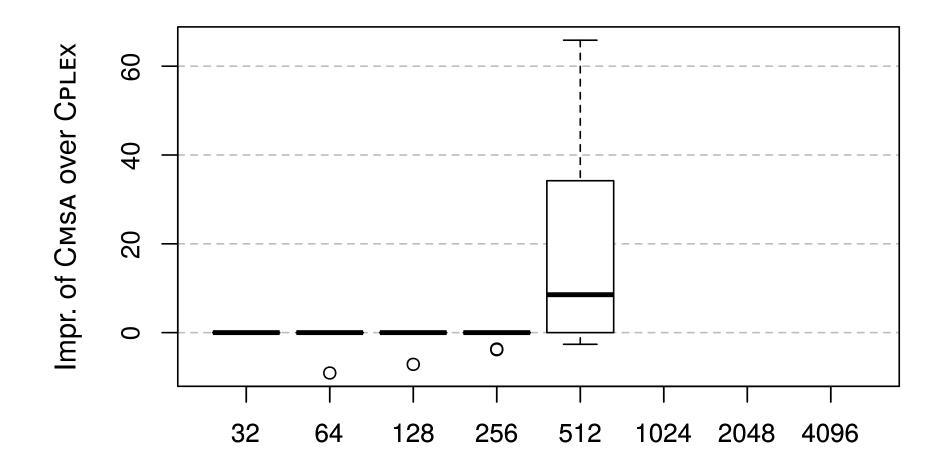
Improvement of CMSA over CPLEX: alphabet size n/8



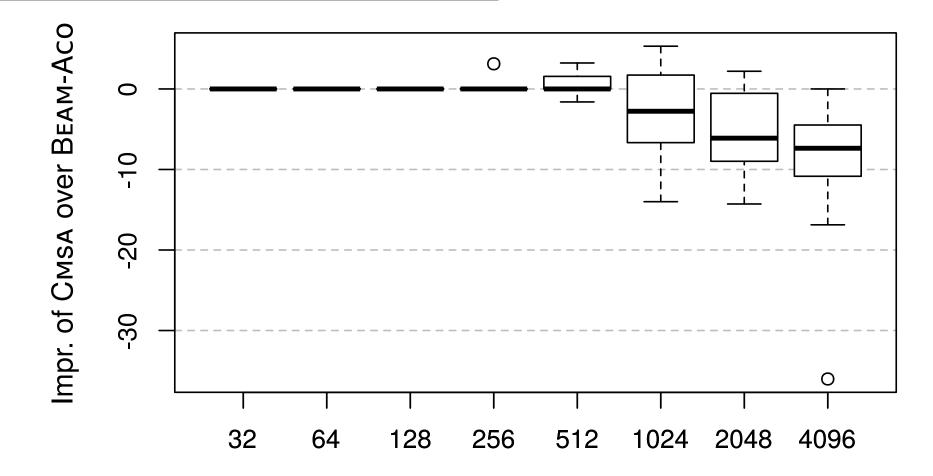
Improvement of CMSA over CPLEX: alphabet size n/2



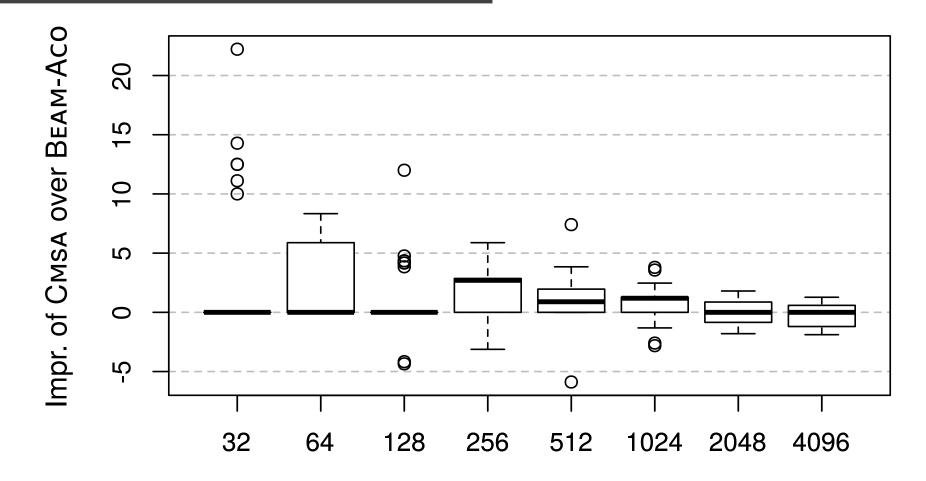
Improvement of CMSA over CPLEX: alphabet size 7n/8



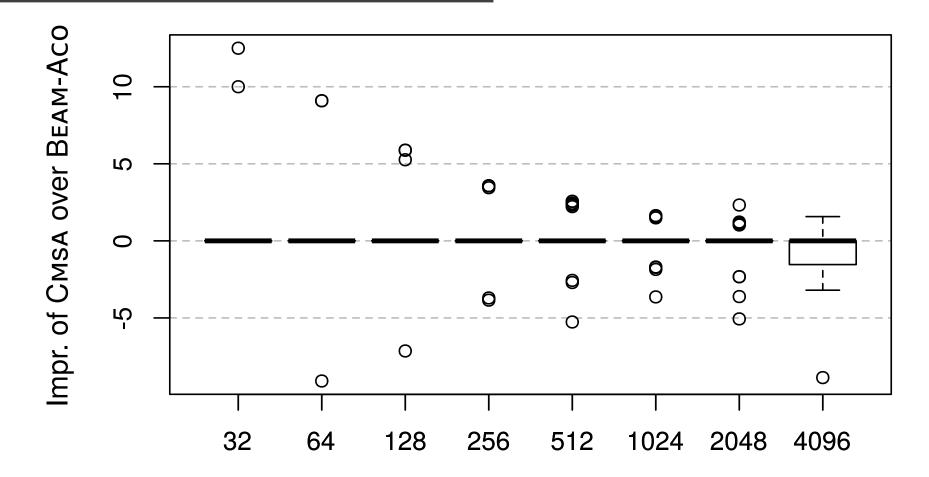
Improvement of CMSA over Beam-ACO: alphabet size n/8



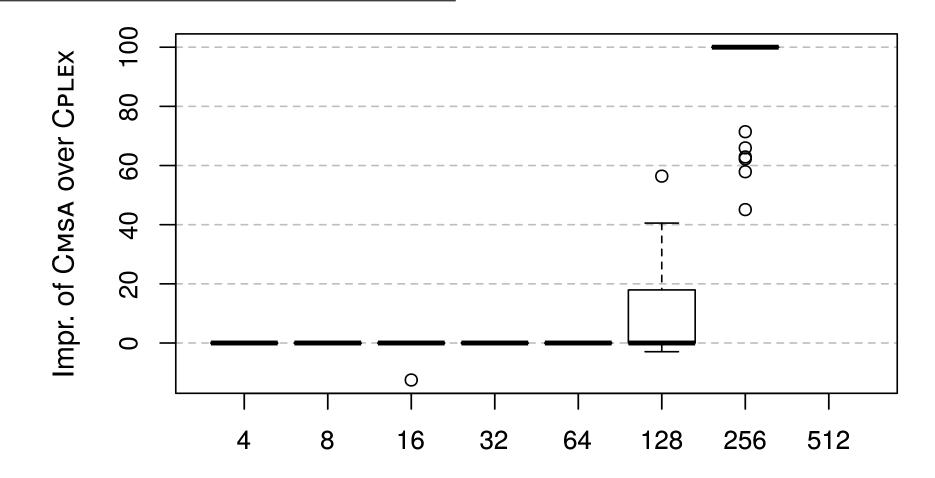
Improvement of CMSA over Beam-ACO: alphabet size n/2



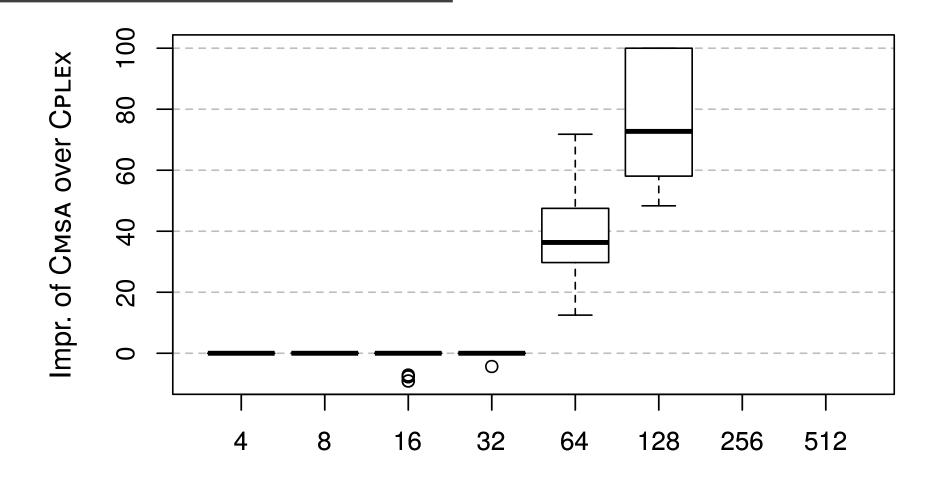
Improvement of CMSA over Beam-ACO: alphabet size 7n/8



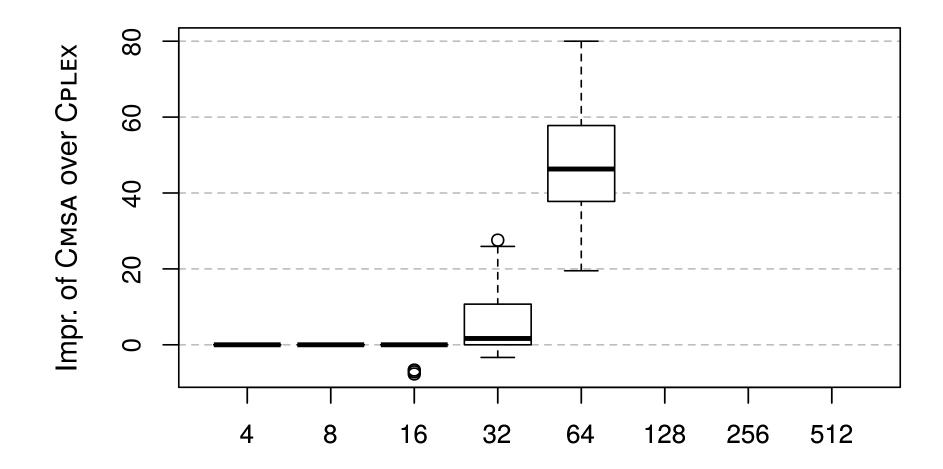
Improvement of CMSA over CPLEX: 3 reps



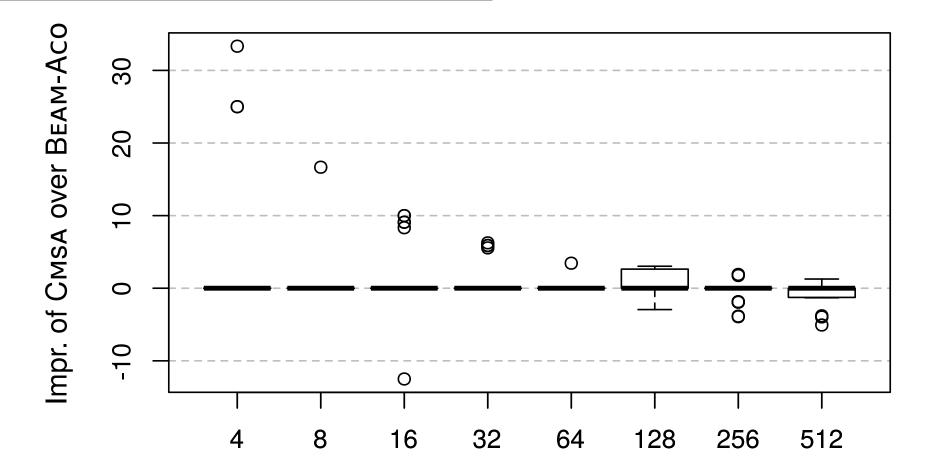
Improvement of CMSA over CPLEX: 6 reps



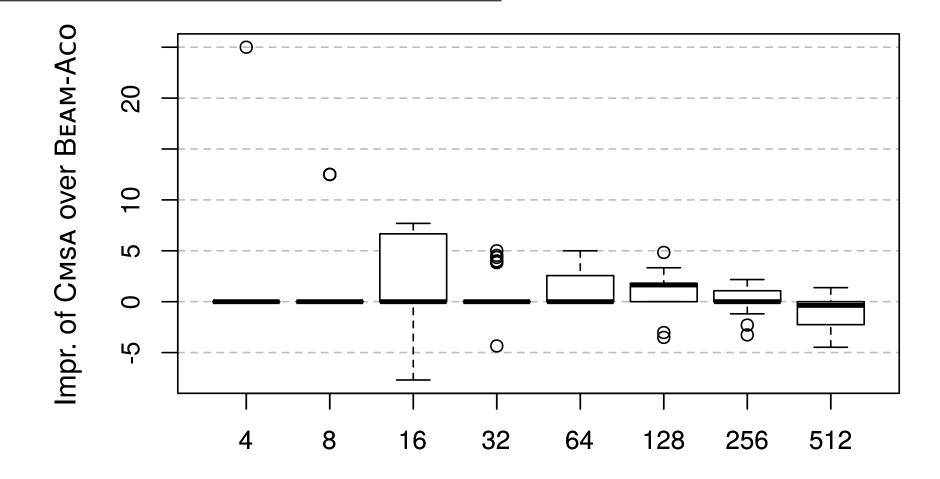
Improvement of CMSA over CPLEX: 8 reps



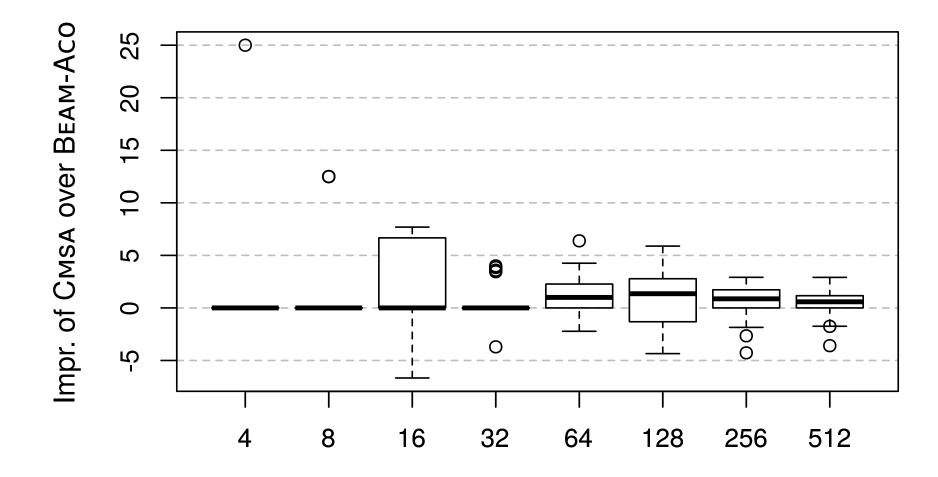
Improvement of CMSA over Beam-ACO: 3 reps



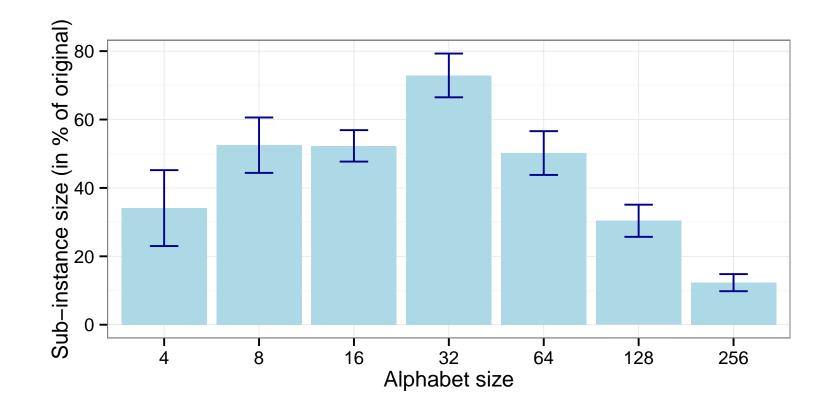
Improvement of CMSA over Beam-ACO: 6 reps



Improvement of CMSA over Beam-ACO: 8 reps



Experimental results: size of sub-instances



Synergy effects: Set1

	10		a /o	/2		0 / 4	
$n \Sigma $	n/8	n/4	3n/8	n/2	5n/8	3n/4	7n/8
32	0.0	0.0	0.0	0.0	0.0	0.0	0.0
64	0.0	0.0	0.0	0.0	0.03	0.0	0.04
128	0.0	0.07	0.0	0.07	0.0	0.0	0.03
256	0.0	-0.07	0.04	0.13	0.03	0.1	0.07
512	-0.14	0.2	0.17	0.27	0.23	0.23	0.14
1024	-0.4	0.47	0.23	0.53	0.03	0.44	0.13
2048	-2.17	0.7	0.5	0.7	0.17	0.73	0.3
4096	-4.16	2.2	0.5	1.14	0.43	1.07	0.67

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Synergy effects: Set2

$reps \Sigma $	4	8	16	32	64	128	256	512
3	0.0	0.0	0.03	0.0	0.0	0.23	0.1	0.3
4	0.0	0.0	0.0	0.0	0.0	0.27	0.23	0.2
5	0.03	0.0	0.0	0.0	0.04	0.16	0.23	0.23
6	0.0	0.0	0.04	0.0	0.04	0.17	0.5	0.3
7	0.0	0.0	0.0	0.0	0.1	0.17	0.57	1.0
8	0.0	0.0	0.1	0.0	0.0	0.44	0.4	0.1

Relation between LNS and CMSA

First experimental study

Reminder: Intuition

▶ CMSA will have advantages over LNS when solutions are small, that is, when

- 1. solutions consist of few solution components
- 2. many variables in the corresponding ILP model have value zero
- ▶ LNS will have advantages over CMSA when the opposite is the case

Problem: how to show this?

- ► Theoretically? hardly possible
- **Empirically?** Maybe with a parametrizable problem

Example: Multi-dimensional Knapsack Problem (MDKP)

Given:

- ► A set of items $C = \{1, ..., n\}$
- ▶ A set of resources $K = \{1, ..., m\}$
- ▶ Of each resource k we have a maximum quantity c_k (capacity)
- ▶ Each item *i* requires from each resource *k* a certain quantity $r_{i,k}$
- \triangleright Each item *i* has a profit p_i

Valid solutions: Each subset $S \in C$ is a valid solution if

$$\sum_{i \in S} r_{i,k} \le c_k \quad \forall k \in K$$

Objective function: $f(S) := \sum_{i \in S} p_i$ for all valid solutions S

MDKP: instance tightness

Important parameter: Instance tightness $0 \le \alpha \le 1$

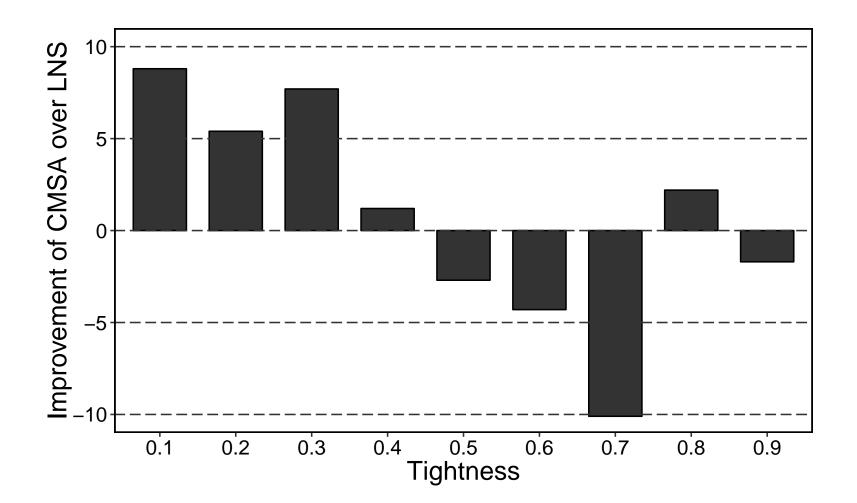
- When α close to zero: capacities are low and valid solution only contain very few items
- When α close to one: capacities are very high and solutions contain nearly all items

Plan:

- ▶ Apply both LNS and CMSA to instances from the whole tightness range.
- Both algorithms are tuned with irace seperately for instances of each considered tightness.

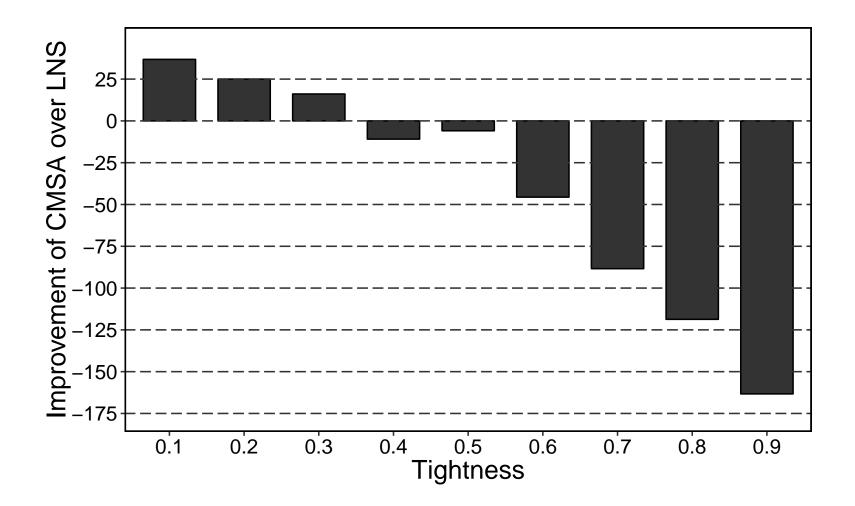
Results for instances with 1000 items

Instance size: n = 1000, m = 10



Results for instances with 5000 items

Instance size: n = 5000, m = 10



Summary and Possible Research Directions

Summary:

- **BEAM-ACO:** Hybrid algorithm combining ACO with beam search
- **CMSA:** A new matheuristic for combinatorial optimization

Possible Research Directions (CMSA):

- **Solution construction:** adaptive probabilities over time
- ► A more intelligent version of the aging mechanism
- ► Taking profit from research on column generation

People involved in certain aspects of this research



Maria J. Blesa



Borja Calvo



Pedro Pinacho



Evelia Lizárraga



Jóse Antonio Lozano

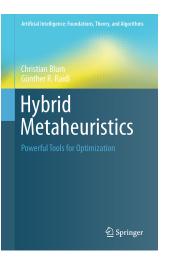


Manuel López-Ibáñez

Questions?

Literature:

- ► C. Blum. Beam-ACO hybridizing ant colony optimization with beam search: an application to open shop scheduling, Computers & OR, 2005
- C. Blum, P. Pinacho, J. A. Lozano, M. López-Ibáñez. Construct, Merge, Solve & Adapt: A new general algorithm for combinatorial optimization. Computers & Operations Research, 2016



New book: C. Blum, G. R. Raidl. Hybrid Metaheuristics – Powerful Tools for Optimization, Springer Series on Artificial Intelligence, 2016