Unsupervised Machine Learning for the Quadratic Assignment Problem

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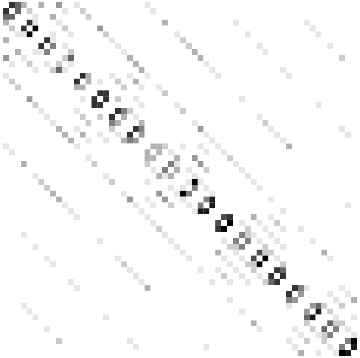
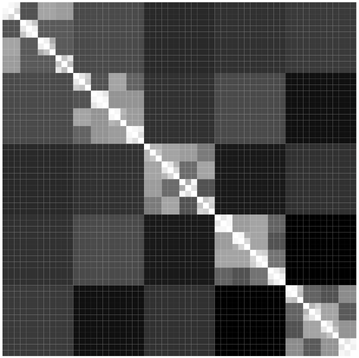
The Quadratic Assignment Problem

First description: [Koopmans and Beckmann(1957)], Monograph: [Çela(1998)]

Definition

- **Data**: Matrices $A = (a_{ij})$ (flows) and $B = (b_{ij})$ (distances), $n \times n$
- **Solution:** A permutation π of $\{1, 2, \ldots, n\}$ (position) of the n items
- **Objective:** $\min_\pi z(\pi) = \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij} b_{\pi(i)\pi(j)}$





“Matrix dot product”

Algorithms for the QAP

- Exact algorithms: $n < 35, 49$
- Constructive algorithms (heuristics)
  - Greedy algorithms not efficient: placing the first item costs nothing; the cost of placing the last item can be arbitrarily large
  - Learning good positions for each item (Ant Systems)
  - Goal of this work: can we learn good positions with locally optimum solutions?
- Local searches
  - Taboo searches (Robust, Reactive)
  - Late Acceptance Hill Climbing
  - With Ant Systems: FANT
  - With Population Management: GA, Path Relinking

Machine Learning : Possible approaches

- Ideally: $2n^2$ inputs $\rightarrow$ n outputs (a good permutation)
  - Far from supervised ML capabilities (even for simpler problems like TSP)
- Unsupervised learning
  - Clustering, k-means
  - Neural networks (various topologies, self-organizing (Kohonen) maps)
  - Principal component analysis
  - Frequent features (itemset) appearing in local optima

Extraction and Combination of Frequent Itemsets

Suppose we have 4 local optimum solutions

position	a	b	c	d	e	f	g	$\dots$
	10	8	7	14	1	13	21	$\dots$
item	2	8	7	5	1	17	11	$\dots$
	10	11	7	13	1	14	24	$\dots$
	9	8	4	7	1	14	24	$\dots$

Supported itemsets (frequency $>$ 25% for this portion):

1-itemset		2-itemset			3-itemset				4-itemset
$1 - e$	(100%)	$1 - e$	$7 - c$	(75%)	$1 - e$	$7 - c$	$8 - b$	(50%)	none
$7 - c$	(75%)	$1 - e$	$8 - b$	(75%)	$1 - e$	$7 - c$	$10 - a$	(50%)	
$8 - b$	(75%)	$1 - e$	$10 - a$	(50%)	$1 - e$	$14 - f$	$24 - g$	(50%)	
$10 - a$	(50%)	$1 - e$	$14 - f$	(50%)					
$14 - f$	(50%)	$1 - e$	$24 - g$	(50%)					
$24 - g$	(50%)	$7 - c$	$8 - b$	(50%)					
		$7 - c$	$10 - a$	(50%)					
		$14 - f$	$24 - g$	(50%)					

Apriori algorithm for the extraction of frequent itemsets

Data: $solutions$, min_sup and $itemsets\_limit$

Result: $all\_itemsets$

$k \leftarrow 1$

$C_k \leftarrow generate\_itemsets(solutions, \emptyset, \emptyset)$

$L_k \leftarrow filter\_itemsets(C_k, min\_sup, \emptyset)$

$all\_itemsets \leftarrow L_k$

while $L_k \neq \emptyset$ **do**

  $C_{k+1} \leftarrow generate\_itemsets(solutions, L_k, L_1)$

  $L_{k+1} \leftarrow filter\_itemsets(C_{k+1}, min\_sup, itemsets\_limit)$

  $all\_itemsets \leftarrow all\_itemsets \cup L_{k+1}$

  $k \leftarrow k + 1$

end

Global algorithm for extraction and combination of frequent itemsets

```
Data: instance_data (Flow and distance matrices), nb_solutions (10,000),
nb_generations (8), min_sup (0.1%) and itemsets_limit (1,000,000 for each k)
Result: solutions
forall i ← 1, . . . , nb_solutions do
    solutions[i] ← random_initialization()
    solutions[i] ← local_search(instance_data, solutions[i])
end
forall generation ← 1, . . . , nb_generations do
    all_itemsets ← extract_itemsets(solutions, min_sup, itemsets_limit) (Apriori algorithm)
    forall i ← 1, . . . , nb_solutions do
        solutions[i] ← combine_itemsets(all_itemsets)
        solutions[i] ← local_search(instance_data, solutions[i])
    end
end
```

Policies for combining itemsets

1. **REFI** Random exploration of all frequent itemsets
   - All itemset that can validly complete a partial solution have the same probability of being chosen

2. **ESFI**
   - An itemset has a probability proportional to its occurrence frequency of being chosen
     - Ant System use a similar construction mechanism: Pheromone trails corresponds to 1-itemsets
     - Tabu search exploits itemsets in the reverse way: 2-itemsets to forbid solutions characteristics, 1-itemsets to diversify the search
     - The cross-over operator in genetic algorithms extracts the largest itemset, then add 1-itemsets

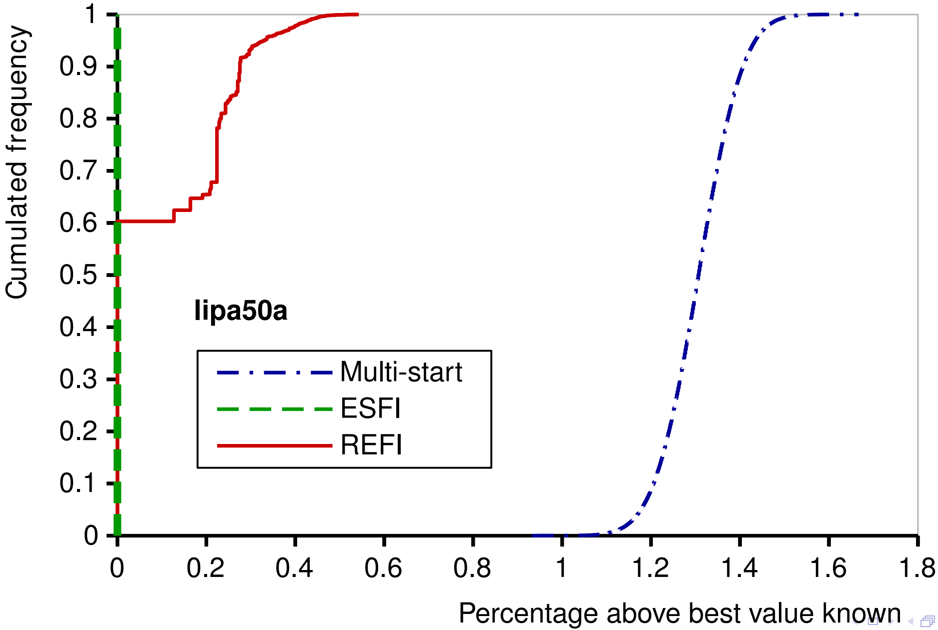
In case a complete solution is not obtained: unassigned items are randomly added

Computational experiments

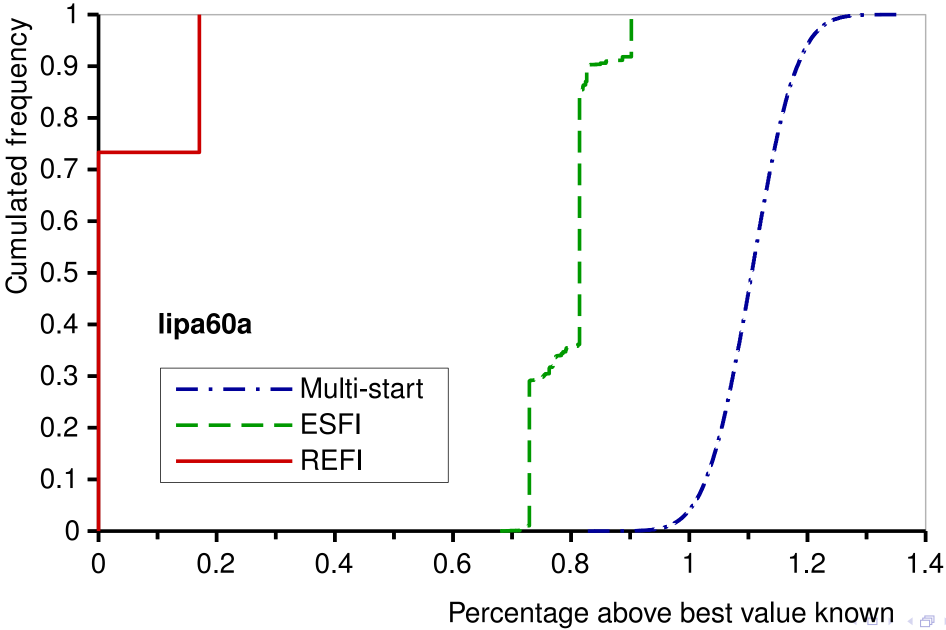
- Computational time
  - Huge
  - About 1 day/generation for $n = 50$ on a CPU with 16 cores (32 threads)
  - The goal was not to design a horse race method

- Instances selection
  - Li and Pardalos : Special generation, known optimum (lipa..a, lipa..b) [Li and Pardalos(1992)]
  - Nugent-Skorin-Kapov : Grid distances, uniform flows (sko..) [Skorin-Kapov(1990)]
  - Symmetric, uniform distances and flows (tai..a) [Taillard(1991)]
  - Asymmetrical, non-uniformly generated (tai..b) [Taillard(1995)]
  - Grey patterns, high number of optimal solutions (tai..c) [Taillard(1995)]
  - Symmetrical and structured (tai..e) [Drezner et al.(2005)Drezner, Hahn, and Taillard]

lipa50a

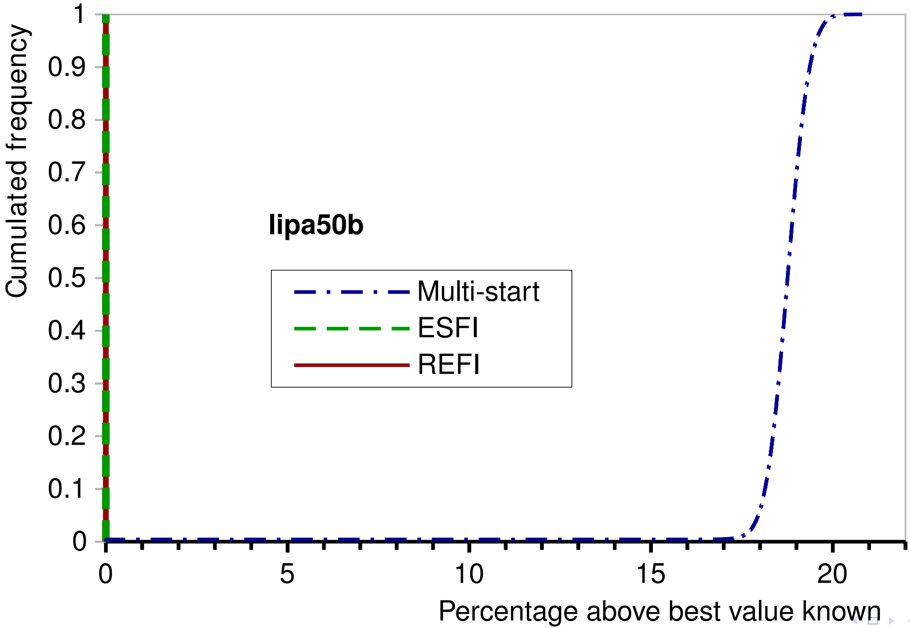

lipa50a
Cumulated frequency
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
Percentage above best value known
Multi-start
ESFI
REFI

lipa60a

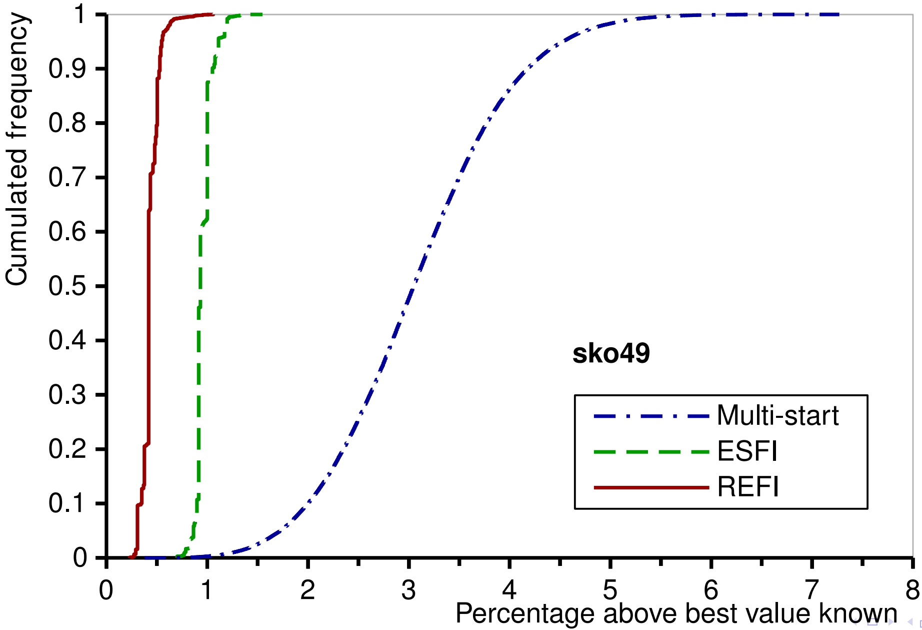


Cumulated frequency
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
lipa60a
Multi-start
ESFI
REFI
0
0.2
0.4
0.6
0.8
1
1.2
1.4
Percentage above best value known

lipa50b

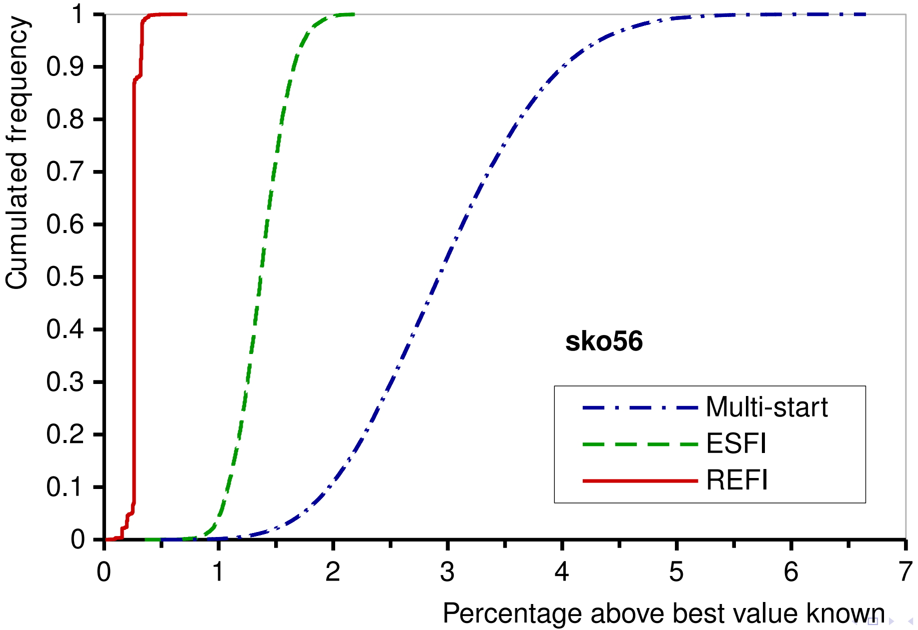

lipa50b
Multi-start
ESFI
REFI
Cumulated frequency
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
5
10
15
20
Percentage above best value known

sko49

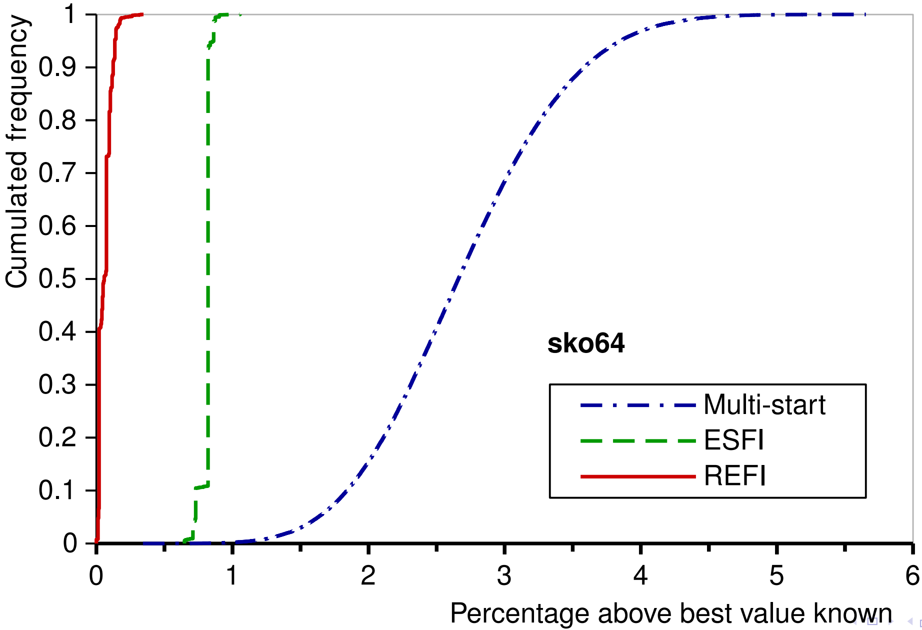


Cumulated frequency
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
1
2
3
4
5
6
7
8
Percentage above best value known
sko49
Multi-start
ESFI
REFI

sko56


sko56
Cumulated frequency
Percentage above best value known
Multi-start
ESFI
REFI
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0
1
2
3
4
5
6
7

sko64



Cumulated frequency
1
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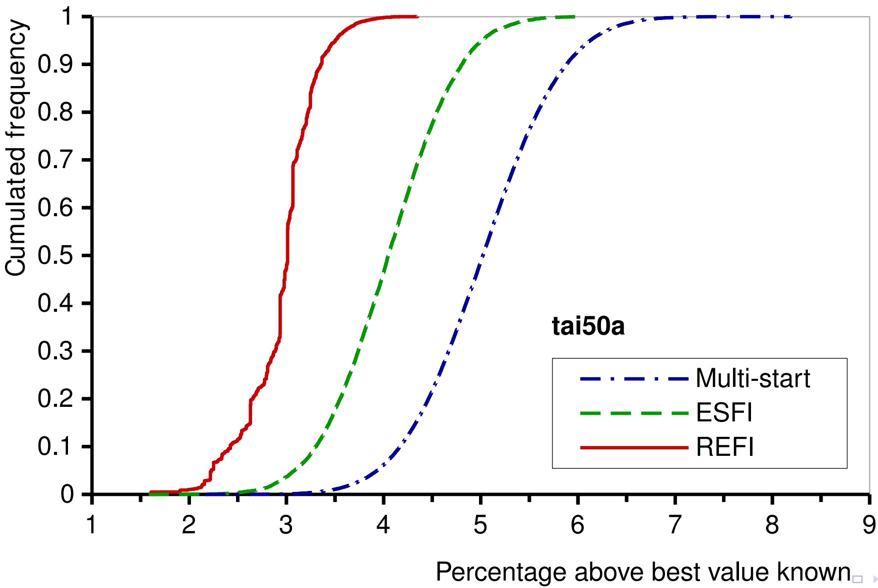
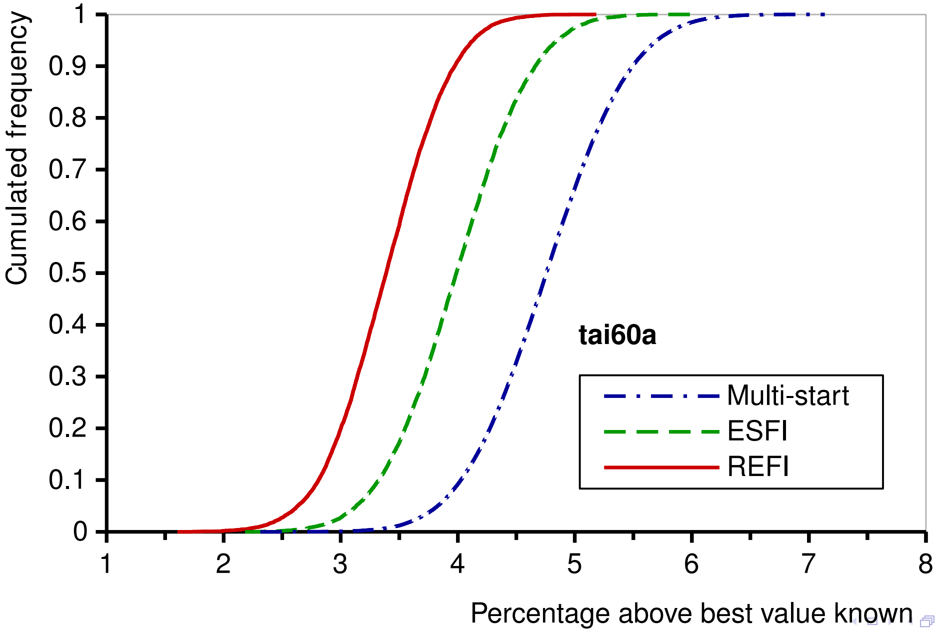
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
1
2
3
4
5
6
Percentage above best value known
sko64
Multi-start
ESFI
REFI

tai50a

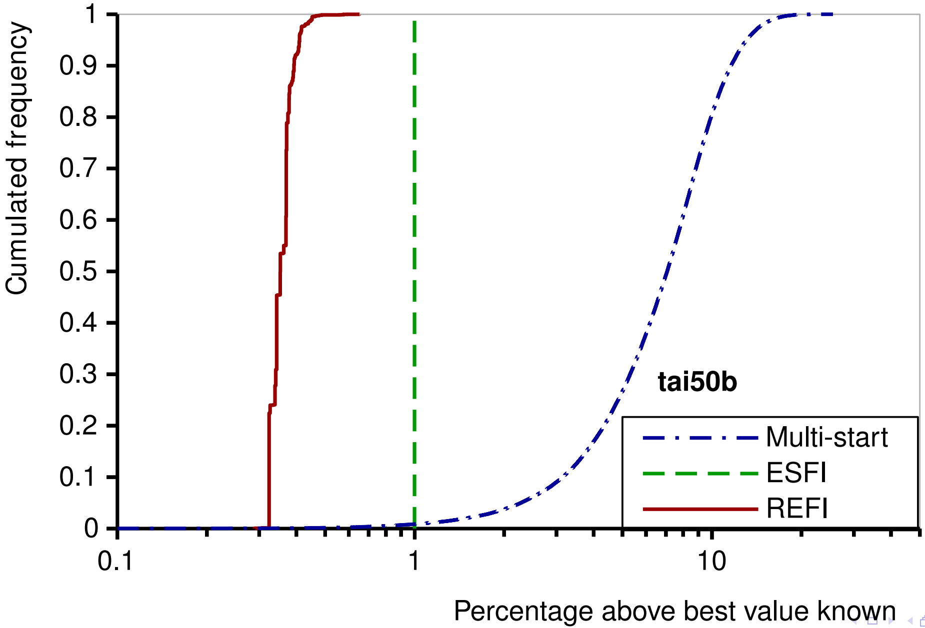


1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
Cumulated frequency
1
2
3
4
5
6
7
8
9
Percentage above best value known
tai50a
Multi-start
ESFI
REFI

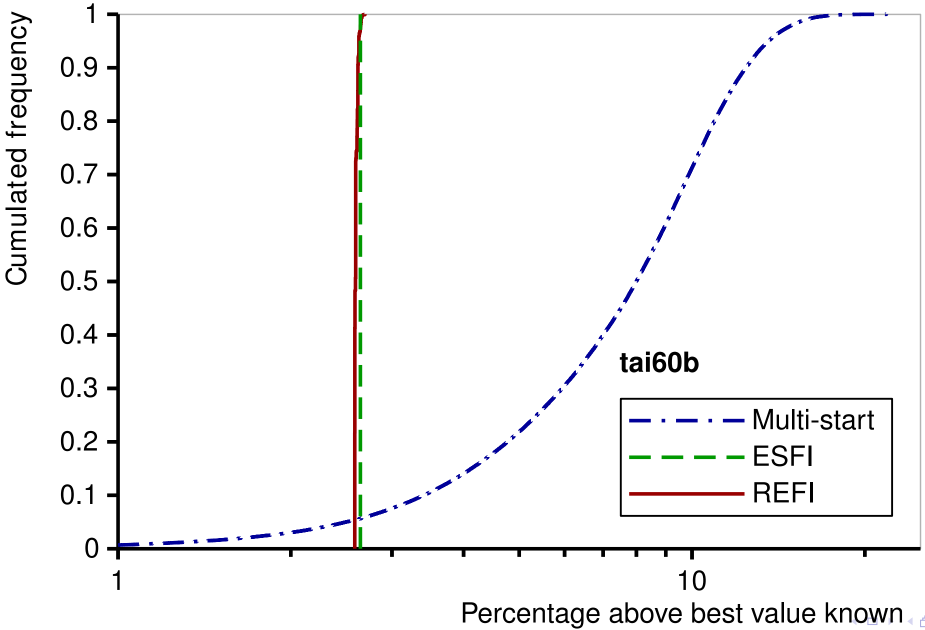
tai60a


Cumulated frequency
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
1
2
3
4
5
6
7
8
Percentage above best value known
tai60a
Multi-start
ESFI
REFI

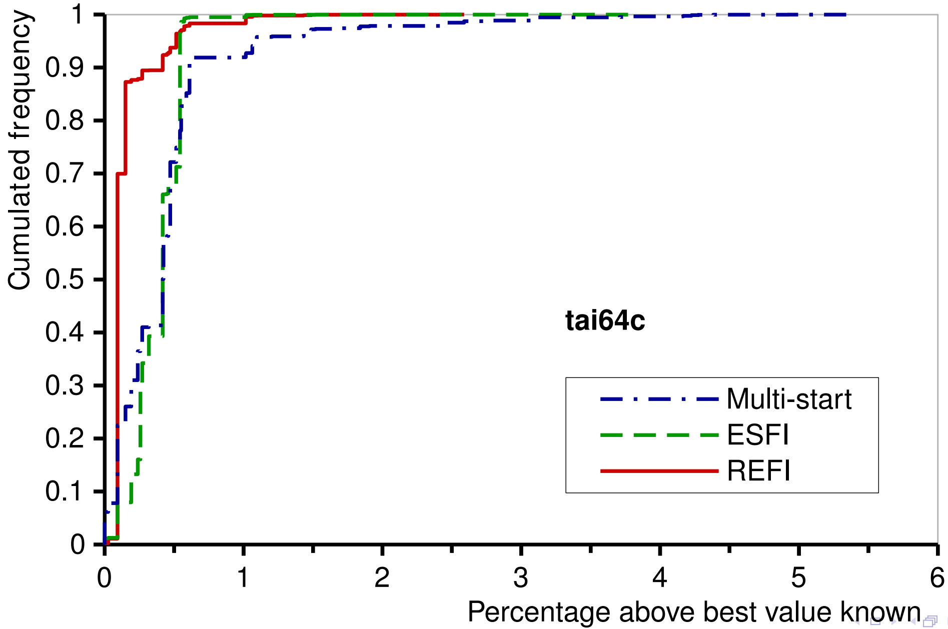
tai50b


Cumulated frequency
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0.1
1
10
tai50b
Multi-start
ESFI
REFI
Percentage above best value known

tai60b

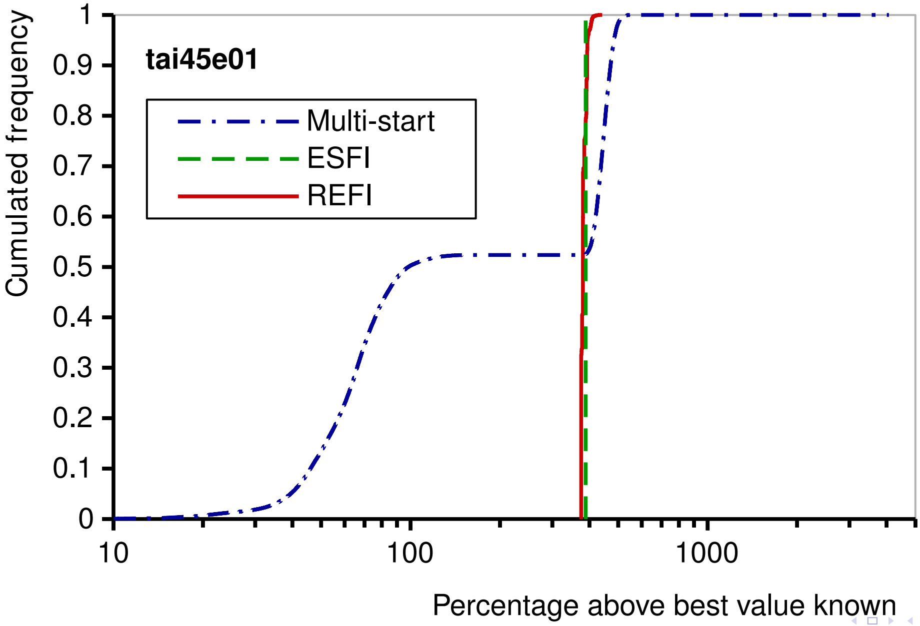

Cumulated frequency
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
1
10
Percentage above best value known
tai60b
Multi-start
ESFI
REFI

tai64c



Cumulated frequency
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
1
2
3
4
5
6
Percentage above best value known
tai64c
Multi-start
ESFI
REFI

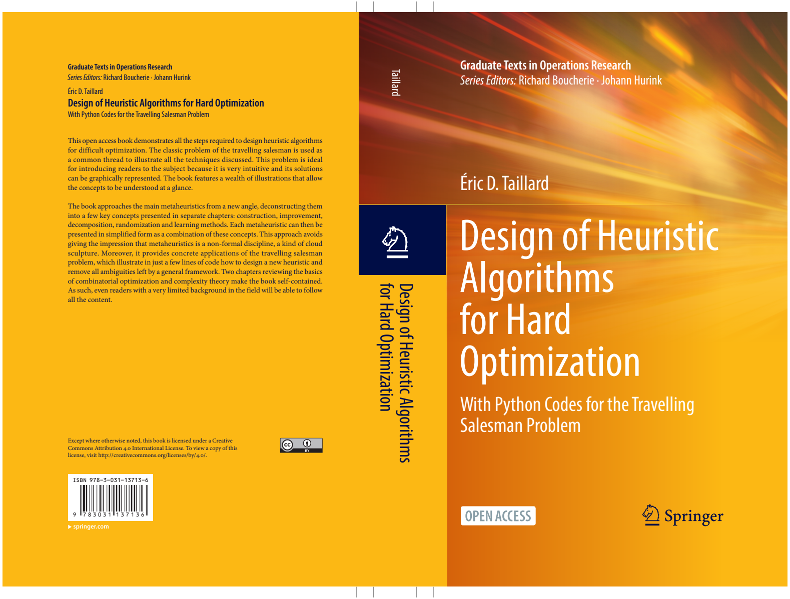
tai45e01


tai45e01
Multi-start
ESFI
REFI
Cumulated frequency
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
10
100
1000
Percentage above best value known

Conclusions

- Independent local searches can hardly find solutions less than 1% above optimum (excepted for tai..c instances)
- REFI is generally better than ESFI
- Building solutions with itemsets frequently found in local optima is efficient for limited instance types (lipa.., sko)
- Unsupervised learning can be highly inefficient for the QAP, even for structured instances
- This contrasts with other problems (for the TSP, a very high fraction of the edges of an optimal solution can be found by few dozen of moderately good solutions [Taillard(2022), Taillard and Heslgaun(2019)])
- A learning mechanism with the supervision of the objective function (as usually done in metaheuristics) is much more efficient. See, e.g. FANT [Taillard(1998)], Ro-TS [Taillard(1991)]

Spam



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