

ML4CO-Bench-101: Benchmark Machine Learning for Classic Combinatorial Problems on Graphs



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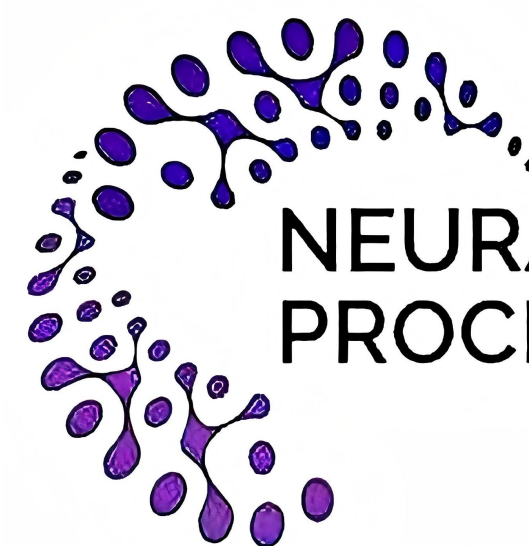
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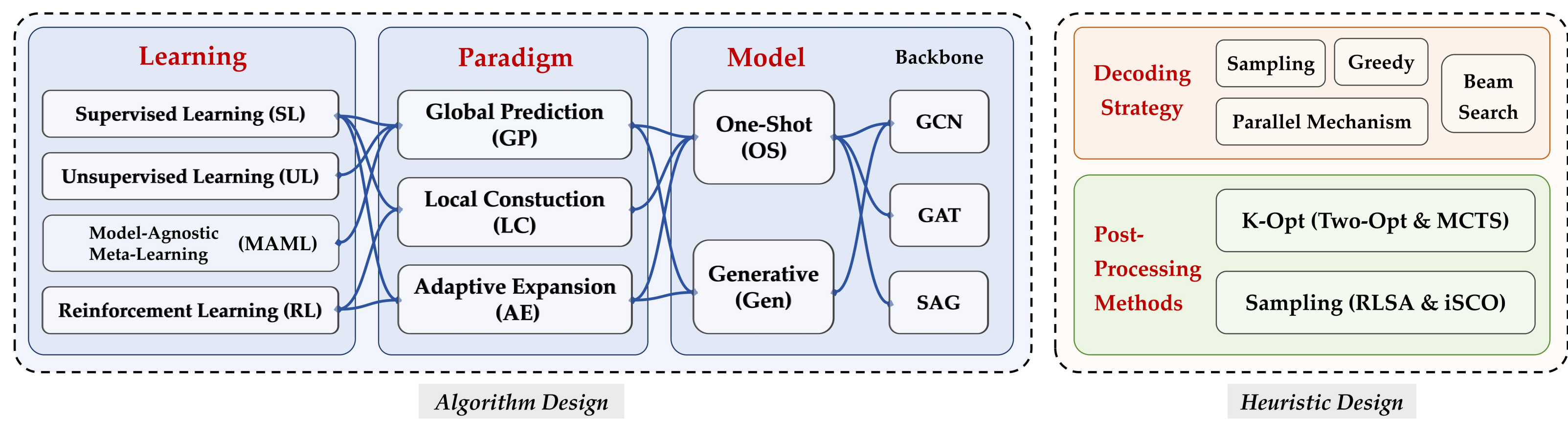
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Benchmark

We provide a detailed analysis of existing methods of ML4CO from: a) *algorithm design*, b) *decoding strategy*, and c) *post-processing optimization*



Algorithm Designs

We compile a collection of representative papers from the past decade that apply machine learning techniques to 7 COPs

Table 1: Categorization of methods: Global Prediction (GP), Local Construction (LC), Adaptive Expansion (AE), Unsupervised/Supervised Learning (U/SL), Model-Agnostic Meta-Learning (MAML).

ID	METHOD	ALGORITHM DESIGN			INVOLVED PROBLEMS						
		PARADIGM	MODEL	LEARNING	TSP	ATSP	CVRP	MIS	MCL	MVC	MCUT
1	Intel [38]	GP	One-Shot	SL	✓	✓	✓	✓	✓	✓	✓
2	GCN [29]	GP	One-Shot	SL	✓	✓	✓	✓	✓	✓	✓
3	Au-GCN [29]	GP	One-Shot	SL	✓	✓	✓	✓	✓	✓	✓
4	GNNGLS [14]	GP	One-Shot	SL	✓	✓	✓	✓	✓	✓	✓
5	GP4CO (Ours)	GP	One-Shot	SL	✓	✓	✓	✓	✓	✓	✓
6	DIMES [18]	GP	One-Shot	MAML (RL)	✓	✓	✓	✓	✓	✓	✓
7	Meta-GCN [20]	GP	One-Shot	MAML (UL)	✓	✓	✓	✓	✓	✓	✓
8	GP4CO (Ours)	GP	One-Shot	MAML	✓	✓	✓	✓	✓	✓	✓
7	UTSP [28]	GP	One-Shot	UL	✓	✓	✓	✓	✓	✓	✓
8	VAG-CO [26]	GP	One-Shot	UL	✓	✓	✓	✓	✓	✓	✓
9	GP4CO (Ours)	GP	One-Shot	UL	✓	✓	✓	✓	✓	✓	✓
9	DiFUSCO [16]	GP	Generative	SL	✓	✓	✓	✓	✓	✓	✓
10	T2T [36] & Fast-T2T [40]	GP	Generative	SL	✓	✓	✓	✓	✓	✓	✓
11	UniCO-MatPOENet [33]	GP	Generative	SL	✓	✓	✓	✓	✓	✓	✓
11	GP4CO (Ours)	GP	Generative	SL	✓	✓	✓	✓	✓	✓	✓
12	DiFUSCO [19]	GP	Generative	UL	✓	✓	✓	✓	✓	✓	✓
13	SDOS [21]	GP	Generative	UL	✓	✓	✓	✓	✓	✓	✓
14	GP4CO (Ours)	GP	Generative	UL	✓	✓	✓	✓	✓	✓	✓
15	RL4CO [41, 45, 30, 42]	LC	One-Shot	RL	✓	✓	✓	✓	✓	✓	✓
16	MaNet [31]	LC	One-Shot	RL	✓	✓	✓	✓	✓	✓	✓
16	UniCO-MatPOENet [33]	LC	One-Shot	RL	✓	✓	✓	✓	✓	✓	✓
17	LC4CO (Ours)	LC	One-Shot	RL	✓	✓	✓	✓	✓	✓	✓
17	BQ-Net [46]	LC	One-Shot	SL	✓	✓	✓	✓	✓	✓	✓
18	GOAL [32]	LC	One-Shot	SL	✓	✓	✓	✓	✓	✓	✓
19	LC4CO (Ours)	LC	One-Shot	SL	✓	✓	✓	✓	✓	✓	✓
19	LwD [43]	AE	One-Shot	RL	✓	✓	✓	✓	✓	✓	✓
20	AE4CO (Ours)	AE	One-Shot	RL	✓	✓	✓	✓	✓	✓	✓
20	COFunder [37]	AE	Generative	SL	✓	✓	✓	✓	✓	✓	✓
21	AE4CO (Ours)	AE	Generative	SL	✓	✓	✓	✓	✓	✓	✓

Decoding & Post-Processing

We compile and implement the most representative decoding and post-processing strategies for 7 COPs

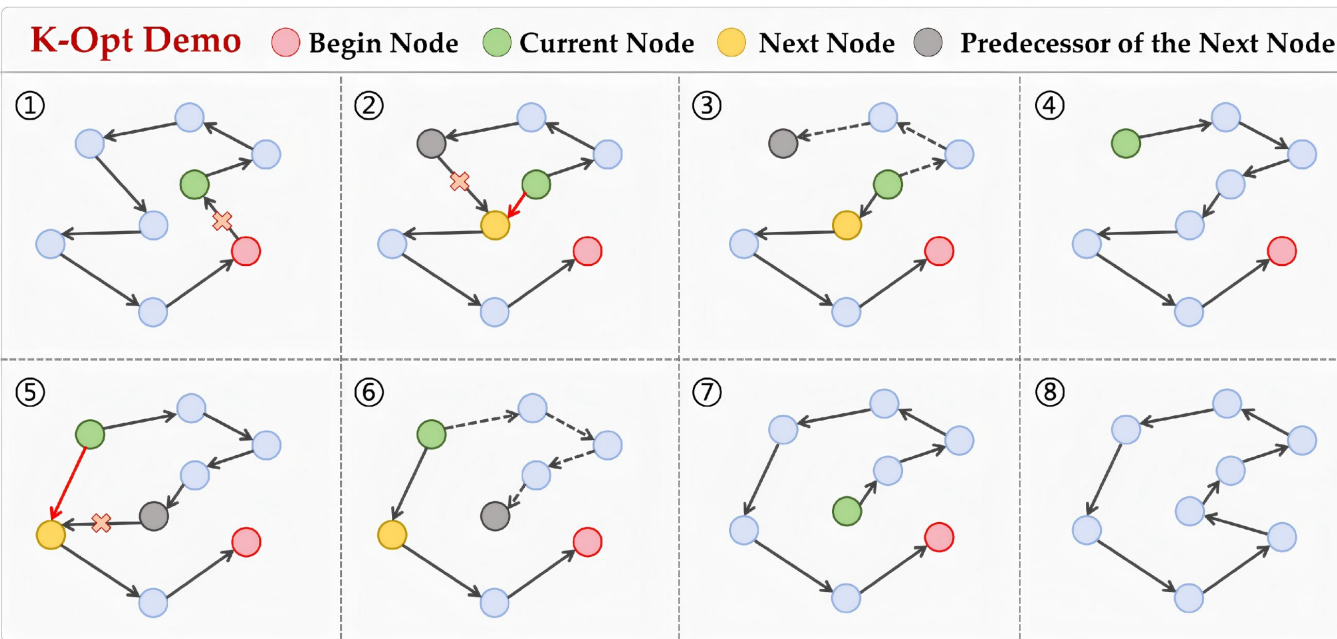


Figure 2: Demonstration of the K-Opt (K=3) post-processing method for TSP.

Algorithm 1 Original RLSA.	Algorithm 2 RLSA as Local Search.
Input: Graph G , Energy Function $H(\cdot)$, hyperparameter $(\tau_0, d, k, l, \alpha_1)$. Initial Solution x_0 . Parallel k. $s \leftarrow \text{Bern}(p = 0.5)$ for $s = 1$ to l do $\tau \leftarrow \tau_0(1 - \frac{s-1}{l-1})$ $\Delta \leftarrow (2k - 1) \odot \nabla H(x)$ for $i = 1$ to N do $p \leftarrow \text{Sigmoid}((\Delta_i - \Delta_{(i)})/(2\tau))$ $c \sim \text{Bern}(p)$ $x_i \leftarrow x_i \cdot (1 - c) + (1 - x_i) \cdot c$ end for if $H(x) < H(x')$ then $x' \leftarrow x$ end for Output: Solution x	Input: Graph G , Energy Function $H(\cdot)$, hyperparameter $(\tau_0, d, k, l, \alpha_1)$. Initial Solution x_0 . Parallel k. $s \leftarrow \text{Bern}(1 - \alpha_2) \cdot x_0 + \alpha_2 \cdot \text{Bern}(p = 0.5)$ for $s = 1$ to l do $\tau \leftarrow \tau_0(1 - \frac{s-1}{l-1})$ $\Delta \leftarrow (2k - 1) \odot \nabla H(x)$ for $i = 1$ to N do $p \leftarrow \text{Sigmoid}((\Delta_i - \Delta_{(i)})/(2\tau))$ $c \sim \text{Bern}(p)$ $x_i \leftarrow x_i \cdot (1 - c) + (1 - x_i) \cdot c$ end for if $H(x) < H(x')$ then $x' \leftarrow x$ end if Output: Solution x

Dataset

We provide the open-source datasets: including 24 train datasets and 65 test datasets



Table 11: Overview of our benchmark datasets for the seven COPs. The “MODEL” column indicates the dataset on which the model is trained. I.e., datasets with the same “TYPE” and “MODEL” is suggested for i.i.d. training-testing, whereas datasets with different “TYPE” and “MODEL” (with “testing” part only) are designed for evaluating the o.o.d. generalization performance of models trained on the corresponding (smaller-scaled, differently distributed, etc.) data. The parentheses indicate the solver parameters used: the maximum solution time for Gurobi, KaMIS and HGS; the maximum trials for LKH. **Blue: Cross-distribution Generalization Dataset.**

ID	PROBLEM	TYPE	MODEL	DATA SIZE	SOLVER	STORAGE	DATA SIZE	SOLVER	OBJ.
1	TSP	Uniform-50	Uniform-50	1280,000	Concorde	2.48GB	1280	Concorde	5.688
2	TSP	Uniform-100	Uniform-100	1280,000	Concorde	4.95GB	1280	Concorde	7.756
3	TSP	Uniform-200	Uniform-200	128,000	Concorde	1.05GB	128	Concorde	10.719
4	TSP	Uniform-500	Uniform-500	64,000	Concorde	1.26GB	128	Concorde	16.546
5	TSP	Uniform-1K	Uniform-1K	64,000	LKH(1000)	2.53GB	128	Concorde	23.118
6	TSP	Uniform-10K	Uniform-10K	6,400	LKH(500)	2.59GB	16	LKH(500)	71.755
7	TSP	TSPLIB	Mixed	—	—	—	49	Concorde	8.062
8	TSP	Cluster-50	Uniform-50	—	—	—	1280	Concorde	3.730
9	TSP	Cluster-100	Uniform-100	—	—	—	1280	Concorde	5.526
10	TSP	Cluster-200	Uniform-200	—	—	—	128	Concorde	6.912
11	TSP	Cluster-500	Uniform-500	—	—	—	128	Concorde	10.723
12	TSP	Gaussian-50	Uniform-50	—	—	—	1280	Concorde	23.840
13	TSP	Gaussian-100	Uniform-100	—	—	—	1280	Concorde	34.031
14	TSP	Gaussian-200	Uniform-200	—	—	—	128	Concorde	48.127
15	TSP	Gaussian-500	Uniform-500	—	—	—	128	Concorde	77.521
16	ATSP	Uniform-50	Uniform-50	640,000	LKH(500)	14.72GB	2500	LKH(1000)	1.5545
17	ATSP	Uniform-100	Uniform-100	128,000	LKH(500)	11.78GB	2500	LKH(1000)	1.5660
18	ATSP	Uniform-200	Uniform-200	32,000	LKH(1000)	11.76GB	1000	LKH(1000)	1.5647
19	ATSP	Uniform-500	Uniform-500	6,400	LKH(1000)	14.70GB	100	LKH(1000)	1.5734
20	ATSP	HCP-50	Uniform-50	—	—	—	2500	—	0.0000
21	ATSP	HCP-100	Uniform-100	—	—	—	2500	—	0.0000
22	ATSP	HCP-200	Uniform-200	—	—	—	100	—	0.0000
23	ATSP	HCP-500	Uniform-500	—	—	—	100	—	0.0000
24	ATSP	SAT-54	Uniform-50	—	—	—	2500	—	0.0000
25	ATSP	SAT-102	Uniform-100	—	—	—	2500	—	0.0000
26	ATSP	SAT-200	Uniform-200	—	—	—	100	—	0.0000
27	ATSP	SAT-507	Uniform-500	—	—	—	100	—	0.0000
28	CVRP	Uniform-50	Uniform-50	1280,000	HGS(1s)	2.83GB	10,000	HGS(1s)	10.366
29	CVRP	Uniform-100	Uniform-100	640,000	HGS(20s)	1.11GB	10,000	HGS(20s)	15.563
30	CVRP	Uniform-200	Uniform-200	128,000	HGS(60s)	1.11GB	10,000	HGS(60s)	19.630
31	CVRP	Uniform-500	Uniform-500	12,800	HGS(360s)	28MB	100	HGS(360s)	37.154
32	CVRP	CVRPLIB	Mixed	—	—	—	70	—	45.183
33	MIS	RB-SMALL	RB-SMALL	64,000	KaMIS(10s)	3.52GB	500	KaMIS(60s)	20.090
34	MIS	RB-LARGE	RB-LARGE	6,400	KaMIS(60s)	4.74GB	500	KaMIS(60s)	43.004
35	MIS	RB-GIANT	RB-LARGE	12,800	KaMIS(60s)	4.74GB	50	KaMIS(60s)	49.260
36	MIS	ER-700-800	ER-700-800	12,800	KaMIS(60s)	7.83GB	128	KaMIS(60s)	44.969
37	MIS	ER-1400-1600	ER-700-800	39,500	KaMIS(60s)	3.75GB	128	KaMIS(60s)	50.938
38	MIS	SATLIB	SATLIB	—	—	—	500	KaMIS(60s)	425.954
39	MIS	HK-SMALL	ER-700-800	—	—	—	500	KaMIS(60s)	79.372
40	MIS	HK-LARGE	ER-700-800	—	—	—	500	KaMIS(60s)	330.946
41	MIS	WS-SMALL	ER-700-800	—	—	—	500	KaMIS(60s)	76.904
42	MIS	WS-LARGE	ER-700-800	—	—	—	500	KaMIS(60s)	262.570
43	MCI	RB-SMALL	RB-SMALL	64,000	Gurobi(60s)	3.42GB	500	Gurobi(60s)	19.082
44	MCI	Twitter	RB-SMALL	—	—	—	195	Gurobi(60s)	14.210
45	MCI	COLLAB	RB-SMALL	—	—	—	1000	Gurobi(60s)	41.113
46	MCI	RB-LARGE	RB-LARGE	6,400	Gurobi(300s)	4.74GB	50	Gurobi(300s)	40.182
47	MCI	RB-GIANT	RB-LARGE	—	—	—	50	Gurobi(300s)	81.520
48	MCI	HK-SMALL	RB-SMALL	—	—	—	500	Gurobi(60s)	6.792
49	MCI	HK-LARGE	RB-SMALL	—	—	—	500	Gurobi(60s)	290.227
50	MCI	WS-SMALL	RB-SMALL	—	—	—	500	Gurobi(60s)	7.164
51	MCI	WS-LARGE	RB-LARGE	—	—	—	500	Gurobi(300s)	5.978
52	MVC	RB-SMALL	RB-SMALL	128,000	Gurobi(60s)	7.01GB	500	Gurobi(60s)	205.764
53	MVC	Twitter	RB-SMALL	—	—	—	195	Gurobi(60s)	45.251
54	MVC	COLLAB	RB-SMALL	—	—	—	1000	Gurobi(60s)	65.086
55	MVC	RB-LARGE	RB-LARGE	6,400	Gurobi(300s)	4.74GB	500	Gurobi(300s)	968.228
56	MVC	RB-GIANT	RB-LARGE	—	—	—	50	Gurobi(300s)	2398.480
57	MVC	HK-SMALL	RB-SMALL	—	—	—	500	Gurobi(60s)	142.506
58	MVC	WS-SMALL	RB-SMALL	—	—	—	500	Gurobi(60s)	154.618
59	MCut	BA-SMALL	BA-SMALL	128,000	Gurobi(60s)	1.78GB	500	Gurobi(60s)	727.844
60	MCut	BA-LARGE	BA-LARGE	128,000	Gurobi(300s)	8.08GB	500	Gurobi(300s)	2936.886
61	MCut	BA-GIANT	BA-LARGE	—	—	—	50	Gurobi(300s)	7217.900
62	MCut	HK-SMALL	BA-SMALL	—	—	—	500	Gurobi(60s)	1540.608
63	MCut	HK-LARGE	BA-LARGE	—	—	—	500	Gurobi(300s)	6401.320
64	MCut	WS-SMALL	BA-SMALL	—	—	—	500	Gurobi(60s)	872.116
65	MCut	WS-LARGE	BA-LARGE	—	—	—	500	Gurobi(300s)	3484.176

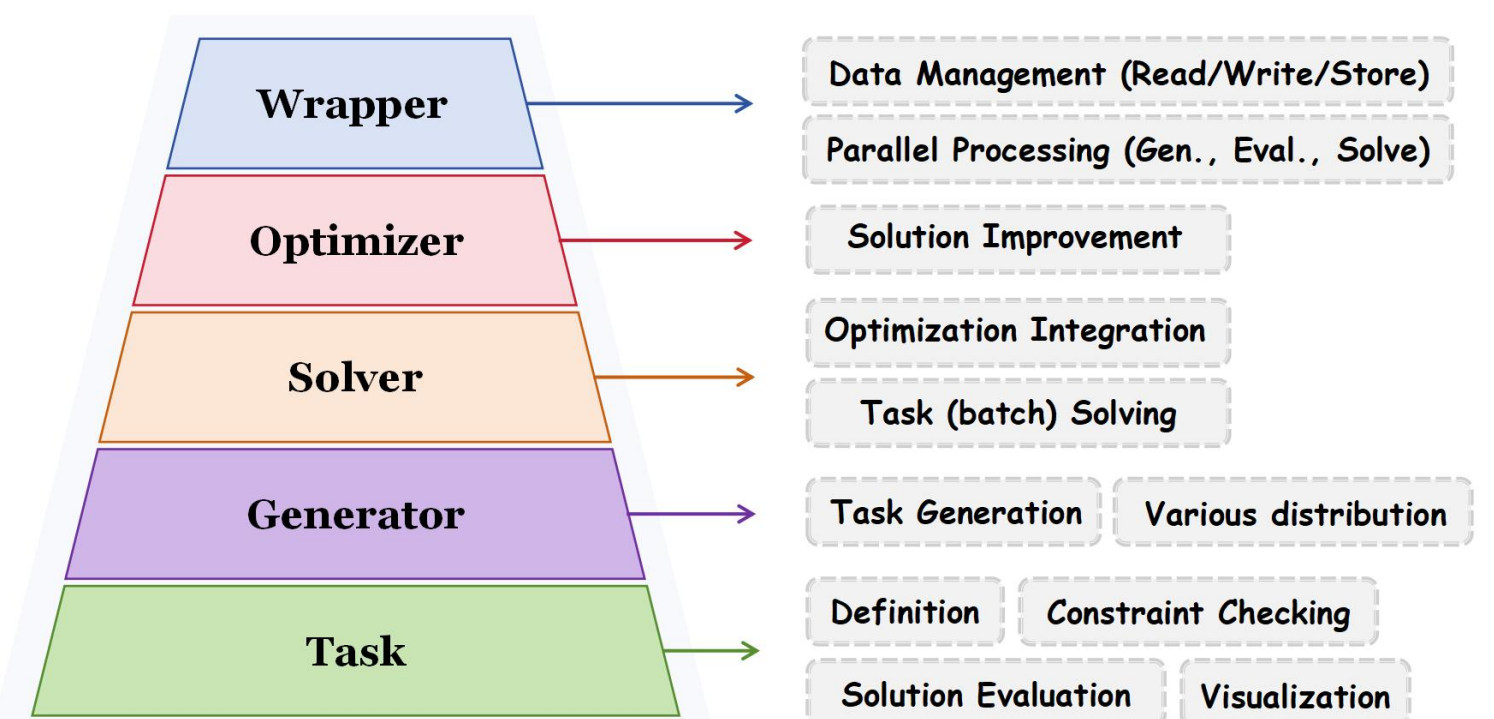
ML4CO-Kit



We have developed the open-source toolkit *ML4CO-Kit*, which aims to provide: decoding or post-processing algorithms, traditional solvers, evaluators, data generators, visualization tools, and read and write functions for various COPs



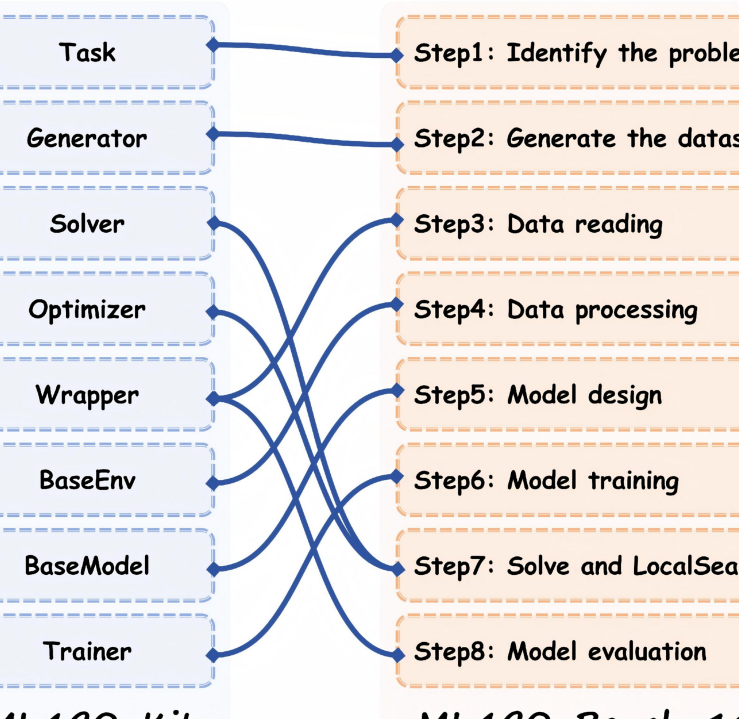
ML4CO-KIT



ML4CO-Bench-101 is based on ML4CO-Kit



ML4CO-KIT



Under active development, Contributions welcome!

Can't make it to the conference in person. Please feel free to reach out to me via github or email: heatingma@sjtu.edu.cn

Experiments

We conduct the following experiments:

- Without any post-processing, we use the simplest *greedy decoding strategy* to directly compare the performance and efficiency of different algorithmic designs
- We analyze the performance and efficiency of various decoding and post-processing strategies, and—taking both into account—present a comprehensive comparison between SOTA ML4CO and traditional solvers on 65 datasets across 7 COPs

Table 8: ML4CO-101 vs baseline solvers: a summarized comparasion. Rd denotes random.

Problem	Dataset	Learning-free Baseline			Learning-based Methods				
		Method	Obj.	Time↓	Method Type	Settings	Obj.	Drop↓	Time↓
TSP	TSP-50	Concorde (67)	5.688	0.059s	GP-OS-SL	Rd-16 + MCTS (0.05s)	5.688	0.001%	0.031s
TSP	TSP-100	Concorde (67)	7.756	0.238s	GP-OS-SL	Rd-16 + MCTS (0.05s)	7.756	0.005%	0.119s
TSP	TSP-500	Concorde (67)	16.546	18.672s	AE-Gen-SL	4×Greedy + Two-Opt	16.588	0.257%	0.695s
TSP	TSP-1K	Concorde (67)	23.118	84.413s	AE-Gen-SL	4×Greedy + Two-Opt	23.271	0.662%	2.609s
TSP	TSP-10K	LKH(500) (6)	71.755	332.758s	AE-Gen-SL	Greedy + Two-Opt	72.832	1.450%	33.485s
TSP	TSPLIB	Concorde (67)	8.062	—	—	—	8.095	0.356%	—
ATSP	ATSP-50	LKH (1K) (6)	1.554	0.097s	AE-Gen-SL	4×Greedy + Two-Opt	1.557	0.171%	0.103s
ATSP	ATSP-100	LKH (1K) (6)	1.566	0.238s	AE-Gen-SL	4×Greedy + Two-Opt	1.581	0.946%	0.516s
ATSP	ATSP-200	LKH (1K) (6)	1.565	0.724s	AE-Gen-SL	4×Greedy + Two-Opt	1.588	1.501%	1.097s
ATSP	ATSP-500	LKH (1K) (6)	1.573	4.376s	AE-Gen-SL	4×Greedy + Two-Opt	1.598	1.568%	6.597s
CVRP	CVRP-50	HGS (69)	10.366	1.005s	LC-OS-RL	N×Sampling + Classic-LS	10.489	1.179%	0.154s
CVRP	CVRP-100	HGS (69)	15.563	20.027s	LC-OS-RL	N×Sampling + Classic-LS	15.822	1.663%	0.203s
CVRP	CVRP-200	HGS (69)	19.630	60.024s	LC-OS-RL	N×Sampling + Classic-LS	20.091	2.359%	0.429s
CVRP	CVRP-500	HGS (69)	37.154	360.376s	LC-OS-RL	Beam-16 + Classic-LS	37.901	2.031%	64.589s
CVRP	CVRPLIB	HGS (69)	45.183	—	LC-OS-RL	N×Sampling + Classic-LS	48.263	5.469%	—
MIS	RB-SMALL	Gurobi (5)	20.090	0.538s	AE-Gen-SL	Greedy + RLSA	20.070	0.093%	0.471s
MIS	RB-LARGE	KaMIS (70)	43.044	56.974s	AE-Gen-SL	Greedy + RLSA	42.400	1.366%	1.816s
MIS	ER-700-800	KaMIS (70)	60.753	96.739s	AE-Gen-SL	Greedy + RLSA	44.984	-0.041%	1.390s
MIS	SATLIB	KaMIS (70)	425.954	24.368s	AE-Gen-SL	Greedy + RLSA	425.316	0.151%	1.775s
MIS	ER-1400-1600	KaMIS (70)	50.938	60.824s	AE-Gen-SL	Greedy + RLSA	50.719	0.418%	4.102s
MIS	RB-GIANT	KaMIS (70)	49.260	60.960s	AE-Gen-SL	Greedy + RLSA	47.880	2.741%	9.909s
MCI	RB-SMALL	Gurobi (5)	19.082	0.900s	GP-OS-SL	Beam-16 + RLSA	19.082	0.000%	0.041s
MCI	RB-LARGE	Gurobi (5)	40.182	276.657s	GP-OS-SL	Beam-16 + RLSA	40.256	-0.275%	0.171s
MCI	TWITTER	Gurobi (5)	14.210	0.276s	GP-OS-SL	Beam-16 + RLSA	14.210	0.000%	0.044s
MCI	COLLAB	Gurobi (5)	42.113	0.063s	GP-OS-SL	Beam-16 + RLSA	42.113	0.000%	0.024s
MCI	RB-GIANT	Gurobi (5)	81.520	3606.201s	GP-OS-SL	Beam-16 + RLSA	85.380	-7.912%	4.342s
MVC	RB-SMALL	Gurobi (5)	205.764	3.340s	AE-Gen-SL	Greedy + RLSA	205.772	0.004%	0.612s
MVC	RB-LARGE	Gurobi (5)	968.228	290.227s	AE-Gen-SL	Greedy + RLSA	968.398	0.018%	1.592s
MVC	TWITTER	Gurobi (5)	85.251	0.133s	AE-Gen-SL	Greedy + RLSA	85.251	0.000%	0.115s
MVC	COLLAB	Gurobi (5)	65.086	0.058s	AE-Gen-SL	Greedy + RLSA	65.086	0.000%	0.158s
MVC	RB-GIANT	Gurobi (5)	2396.780	60.612s	AE-Gen-SL	Greedy + RLSA	2397.360	0.026%	8.590s
McCut	BA-SMALL	Gurobi (5)	727.844	60.612s	AE-Gen-SL	Greedy + RLSA	729.706	-0.260%	0.727s
McCut	BA-LARGE	Gurobi (5)	2936.886	300.214s	GP-Gen-SL	Greedy + RLSA	2994.118	-1.932%	0.999s
McCut	BA-GIANT	Gurobi (5)	7217.900	3601.342s	GP-Gen-SL	Greedy + RLSA	7389.300	-2.383%	2.228s