Neural Combinatorial Optimization with Heavy Decoder: Toward Large Scale Generalization

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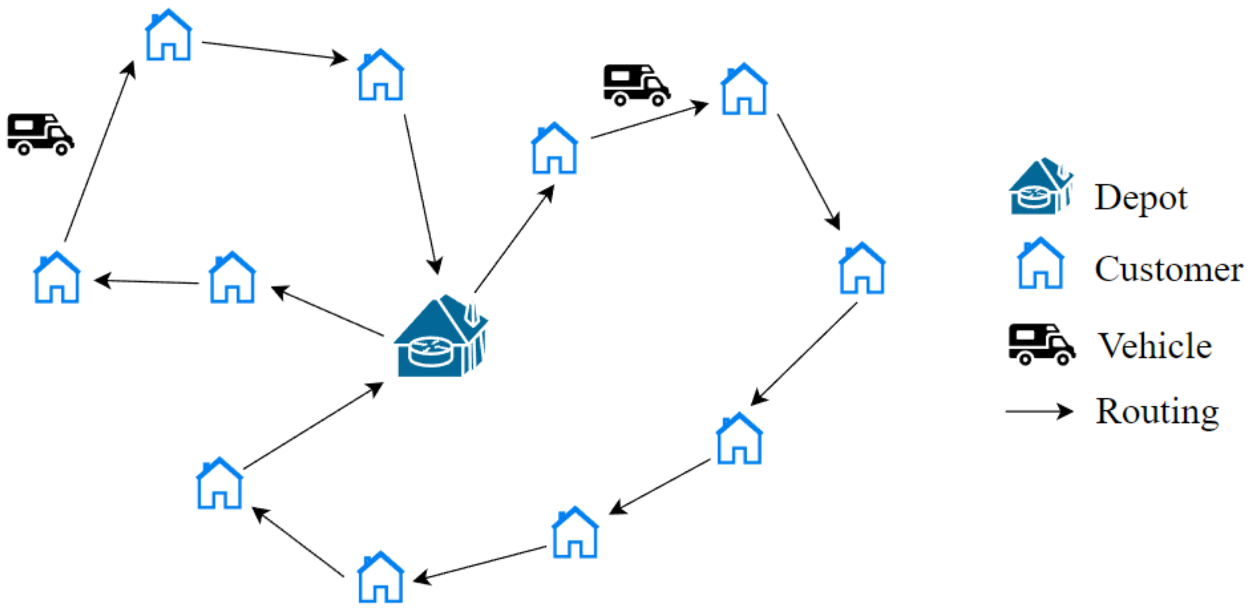
Combinatorial Optimization



Capacitated Vehicle Routing problem

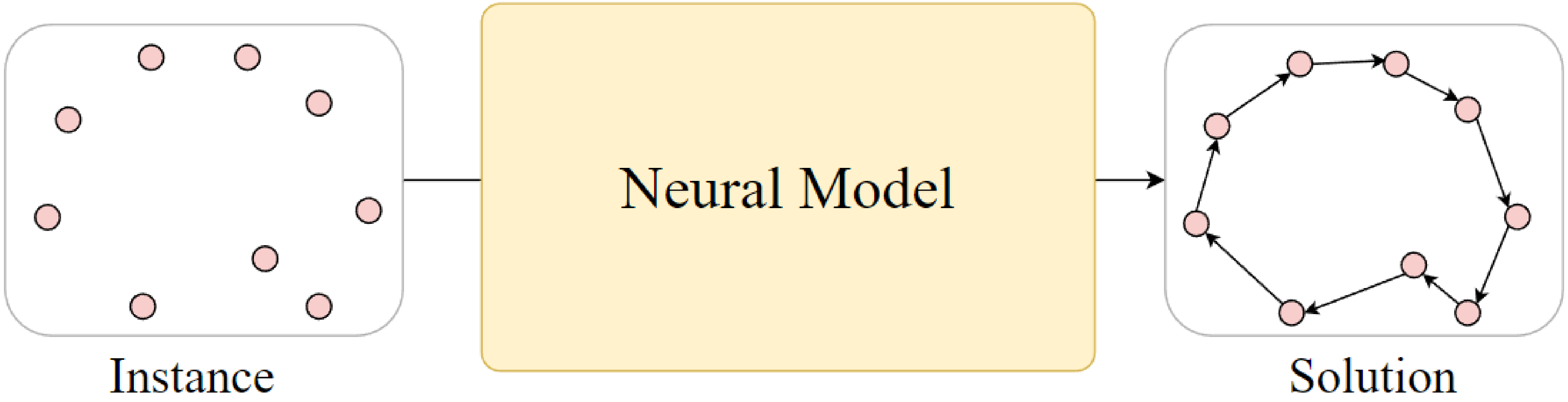
- Combinatorial Optimization

  Vehicle routing, Production planning, Drug discovery, etc.

- Classical Methods

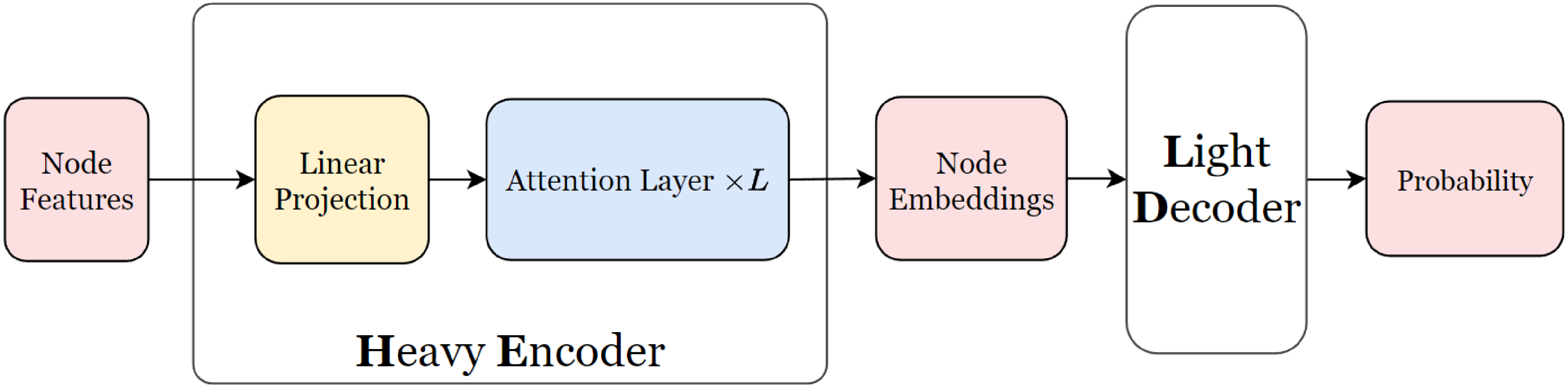
  handcrafted algorithm design, excessively long runtime.

Neural Combinatorial Optimization (NCO)



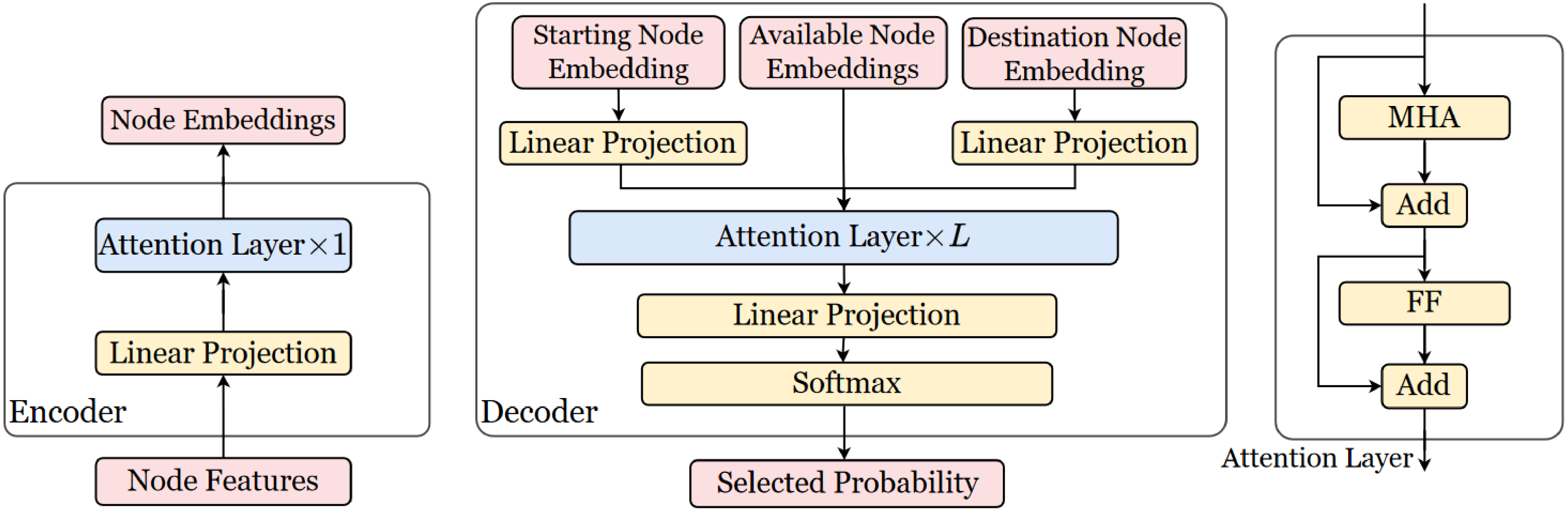
- NCO Methods: No expert design required.
- Limitation: Poor generalization ability.

Motivation



- Existing methods employ the **H**eavy **E**ncoder and **L**ight **D**ecoder structure.
- The heavy encoder tends to learn scale-related features and the light decoder cannot capture dynamically changing relationships of nodes during decoding process, resulting in **poor generalization ability**

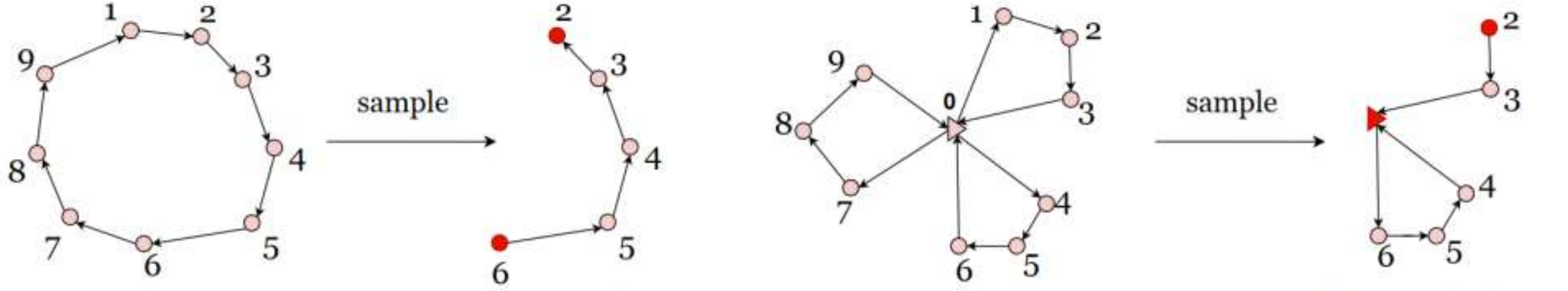
This Work: Light Encoder and Heavy Decoder (LEHD) model



- Heavy decoder dynamically refines and updates relationships among nodes via L attention layers, making more informed node selections for various-sized problem instances.
- Node sizes vary during construction, leading to scale-independent feature learning.

Training Scheme: Learn to Construct Partial Solution

- Generate the Partial Solution

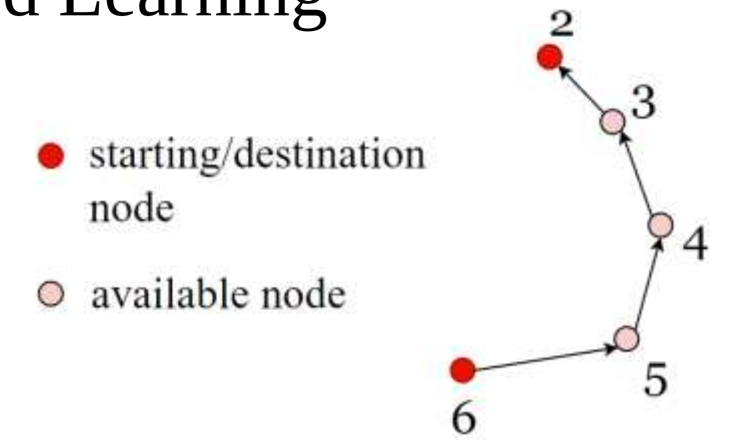


TSP solution TSP partial solution CVRP solution CVRP partial solution

- Learn to Construct Partial Solutions via Supervised Learning

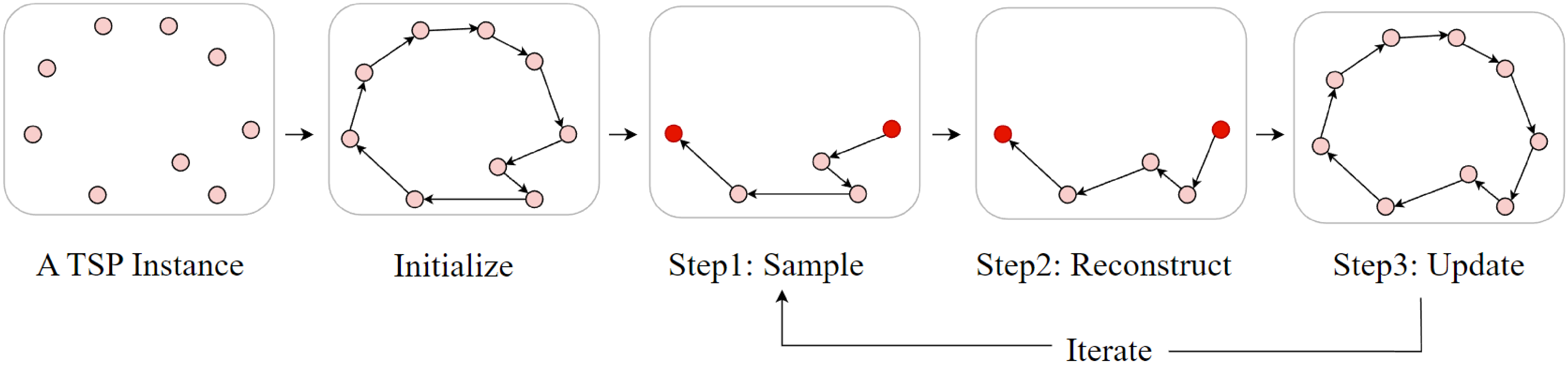
Cross-entropy loss: $loss = -\sum_{i=1}^{u} y_i \log(p_i)$,

- p_i is the selected probability of node i,
- $y_i \in \{0, 1\}$ is the label,
- u is the number of available nodes.



partial solution

Inference Method: Random Re-Construct (RRC)

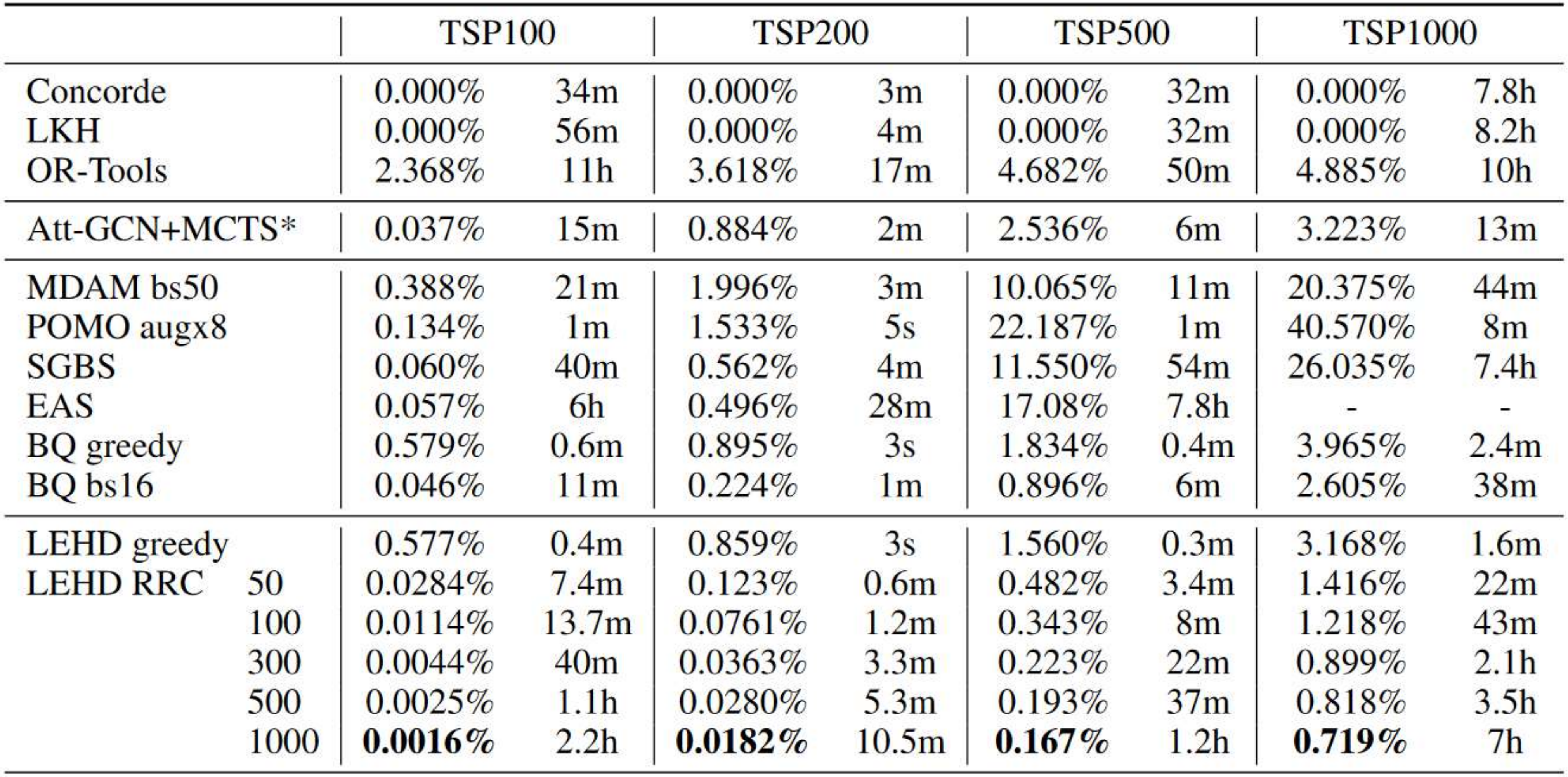


Generate the initial complete solution using Greedy rollout.

- Step1: Randomly **samples** a partial solution from the complete solution.
- Step2: **Reconstructs** the partial solution to obtain a new partial solution.
- Step3: If the new partial solution is superior, it **replaces** the old one.

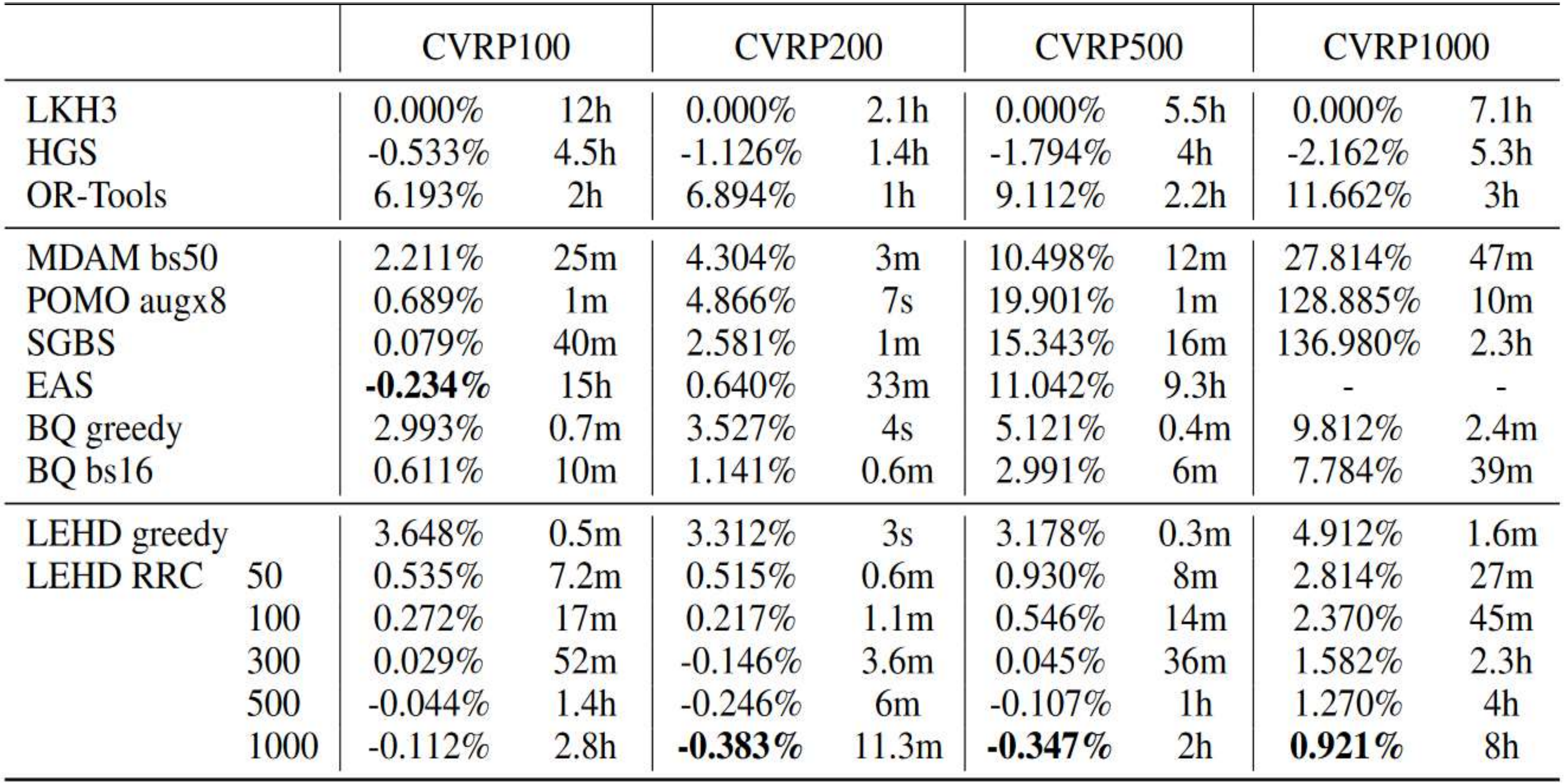
Repeat step 1~3 within a stipulated time budget.

Performance On Uniformly Distributed Instances



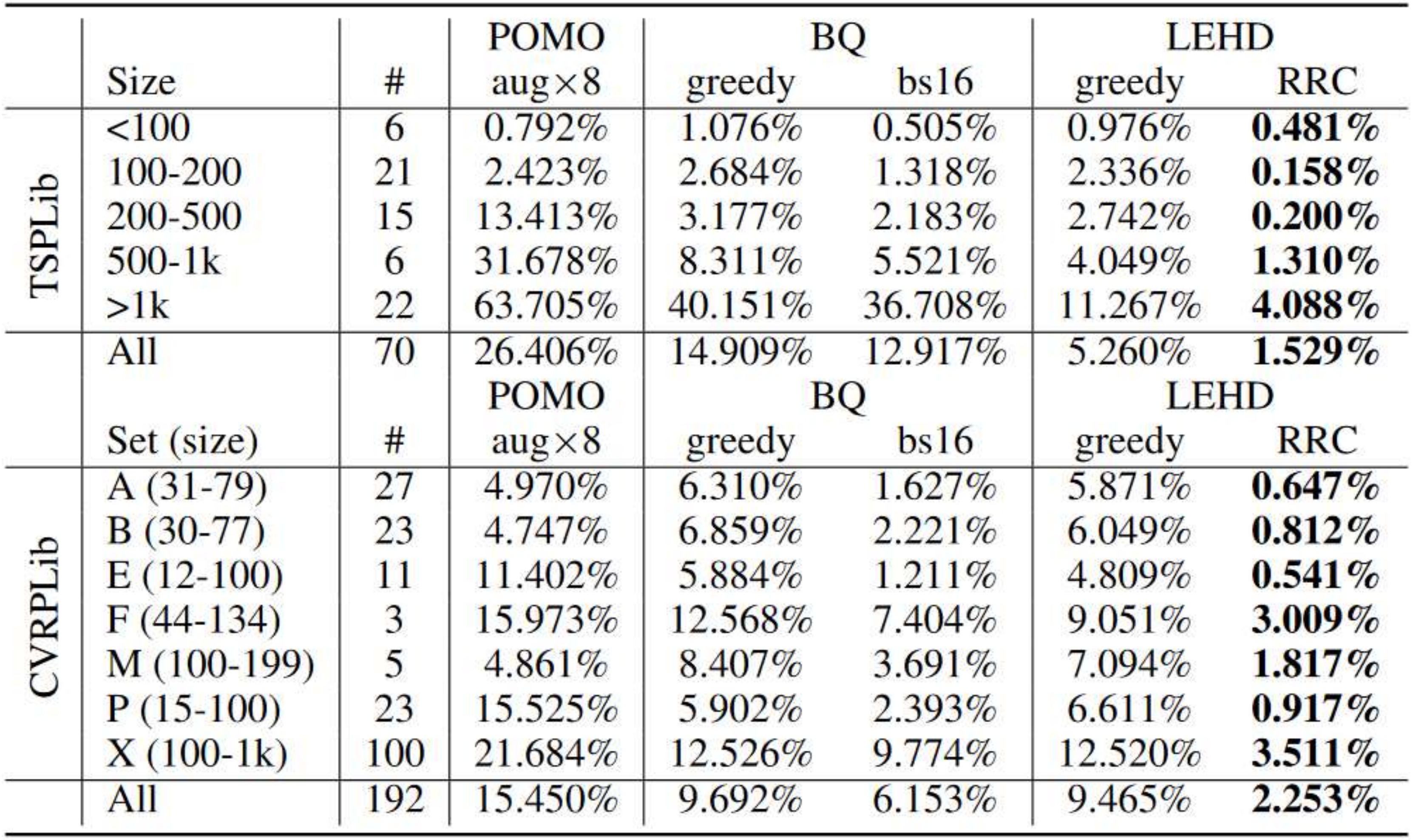
		TSP100		TSP200		TSP500		TSP1000	
Concorde		0.000%	34m	0.000%	3m	0.000%	32m	0.000%	7.8h
LKH		0.000%	56m	0.000%	4m	0.000%	32m	0.000%	8.2h
OR-Tools		2.368%	11h	3.618%	17m	4.682%	50m	4.885%	10h
Att-GCN+MCTS*		0.037%	15m	0.884%	2m	2.536%	6m	3.223%	13m
MDAM bs50		0.388%	21m	1.996%	3m	10.065%	11m	20.375%	44m
POMO augx8		0.134%	1m	1.533%	5s	22.187%	1m	40.570%	8m
SGBS		0.060%	40m	0.562%	4m	11.550%	54m	26.035%	7.4h
EAS		0.057%	6h	0.496%	28m	17.08%	7.8h	-	-
BQ greedy		0.579%	0.6m	0.895%	3s	1.834%	0.4m	3.965%	2.4m
BQ bs16		0.046%	11m	0.224%	1m	0.896%	6m	2.605%	38m
LEHD greedy		0.577%	0.4m	0.859%	3s	1.560%	0.3m	3.168%	1.6m
LEHD RRC	50	0.0284%	7.4m	0.123%	0.6m	0.482%	3.4m	1.416%	22m
	100	0.0114%	13.7m	0.0761%	1.2m	0.343%	8m	1.218%	43m
	300	0.0044%	40m	0.0363%	3.3m	0.223%	22m	0.899%	2.1h
	500	0.0025%	1.1h	0.0280%	5.3m	0.193%	37m	0.818%	3.5h
	1000	**0.0016%**	2.2h	**0.0182%**	10.5m	**0.167%**	1.2h	**0.719%**	7h

Performance On Uniformly Distributed Instances



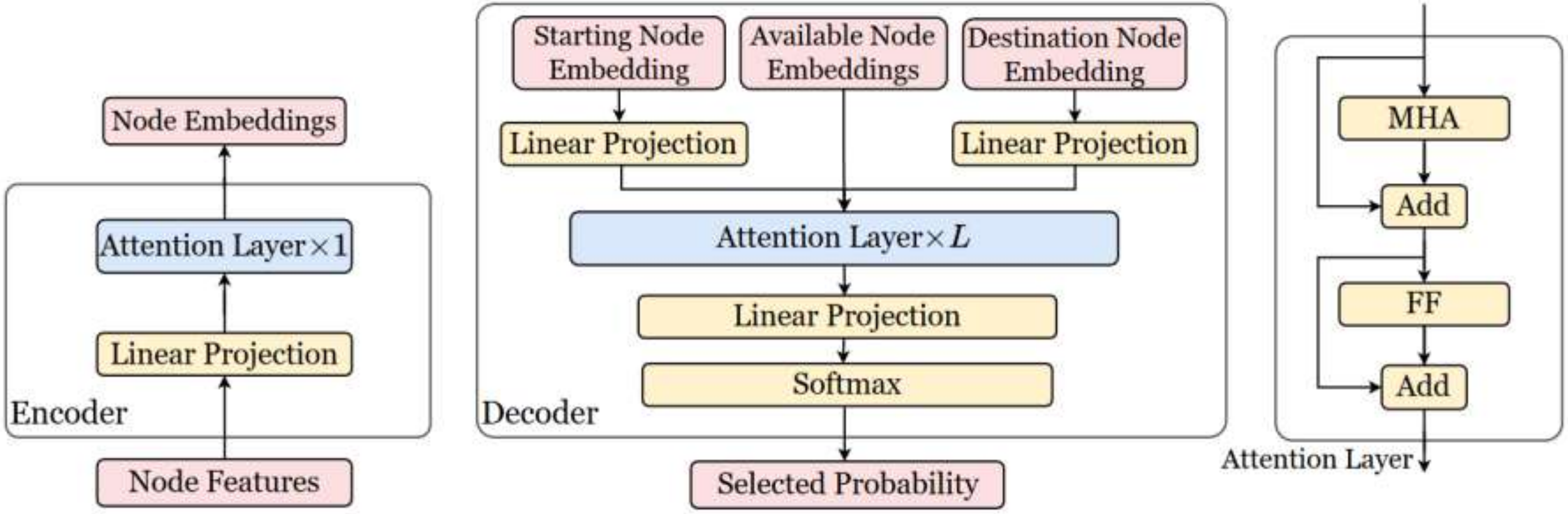
		CVRP100		CVRP200		CVRP500		CVRP1000	
LKH3		0.000%	12h	0.000%	2.1h	0.000%	5.5h	0.000%	7.1h
HGS		-0.533%	4.5h	-1.126%	1.4h	-1.794%	4h	-2.162%	5.3h
OR-Tools		6.193%	2h	6.894%	1h	9.112%	2.2h	11.662%	3h
MDAM bs50		2.211%	25m	4.304%	3m	10.498%	12m	27.814%	47m
POMO augx8		0.689%	1m	4.866%	7s	19.901%	1m	128.885%	10m
SGBS		0.079%	40m	2.581%	1m	15.343%	16m	136.980%	2.3h
EAS		**-0.234%**	15h	0.640%	33m	11.042%	9.3h	-	-
BQ greedy		2.993%	0.7m	3.527%	4s	5.121%	0.4m	9.812%	2.4m
BQ bs16		0.611%	10m	1.141%	0.6m	2.991%	6m	7.784%	39m
LEHD greedy		3.648%	0.5m	3.312%	3s	3.178%	0.3m	4.912%	1.6m
LEHD RRC	50	0.535%	7.2m	0.515%	0.6m	0.930%	8m	2.814%	27m
	100	0.272%	17m	0.217%	1.1m	0.546%	14m	2.370%	45m
	300	0.029%	52m	-0.146%	3.6m	0.045%	36m	1.582%	2.3h
	500	-0.044%	1.4h	-0.246%	6m	-0.107%	1h	1.270%	4h
	1000	-0.112%	2.8h	**-0.383%**	11.3m	**-0.347%**	2h	**0.921%**	8h

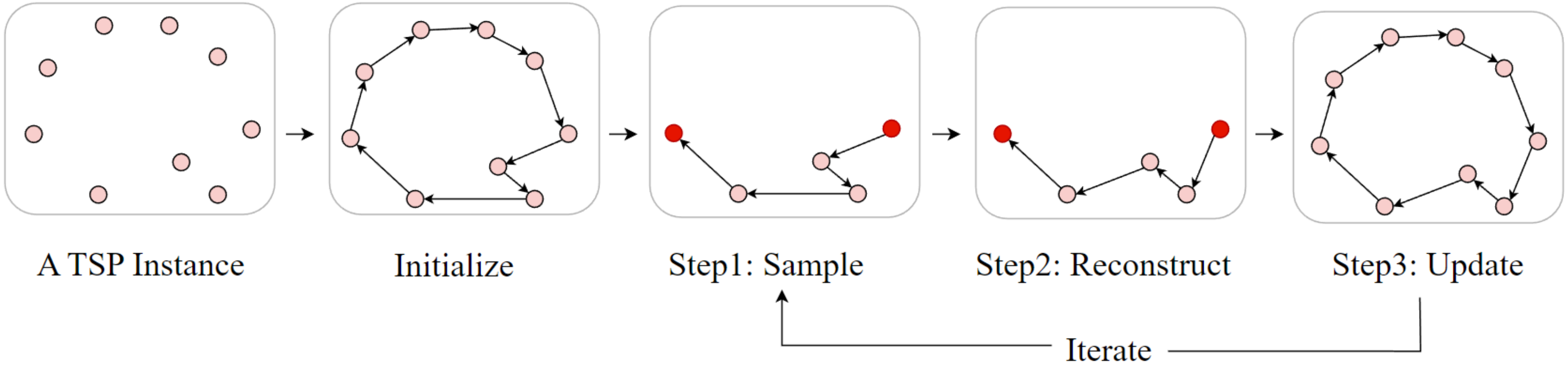
Performance On Real-World Instances



			POMO	BQ		LEHD	
	Size	#	aug×8	greedy	bs16	greedy	RRC
TSPLib	<100	6	0.792%	1.076%	0.505%	0.976%	**0.481%**
	100-200	21	2.423%	2.684%	1.318%	2.336%	**0.158%**
	200-500	15	13.413%	3.177%	2.183%	2.742%	**0.200%**
	500-1k	6	31.678%	8.311%	5.521%	4.049%	**1.310%**
	>1k	22	63.705%	40.151%	36.708%	11.267%	**4.088%**
	All	70	26.406%	14.909%	12.917%	5.260%	**1.529%**
			POMO	BQ		LEHD	
	Set (size)	#	aug×8	greedy	bs16	greedy	RRC
CVRPLib	A (31-79)	27	4.970%	6.310%	1.627%	5.871%	**0.647%**
	B (30-77)	23	4.747%	6.859%	2.221%	6.049%	**0.812%**
	E (12-100)	11	11.402%	5.884%	1.211%	4.809%	**0.541%**
	F (44-134)	3	15.973%	12.568%	7.404%	9.051%	**3.009%**
	M (100-199)	5	4.861%	8.407%	3.691%	7.094%	**1.817%**
	P (15-100)	23	15.525%	5.902%	2.393%	6.611%	**0.917%**
	X (100-1k)	100	21.684%	12.526%	9.774%	12.520%	**3.511%**
	All	192	15.450%	9.692%	6.153%	9.465%	**2.253%**

Summary





- LEHD model
- Learn to Construct Partial Solution
- Random Re-Construct