UniCO: On Unified Combinatorial Optimization via Problem Reduction to Matrix-Encoded General TSP

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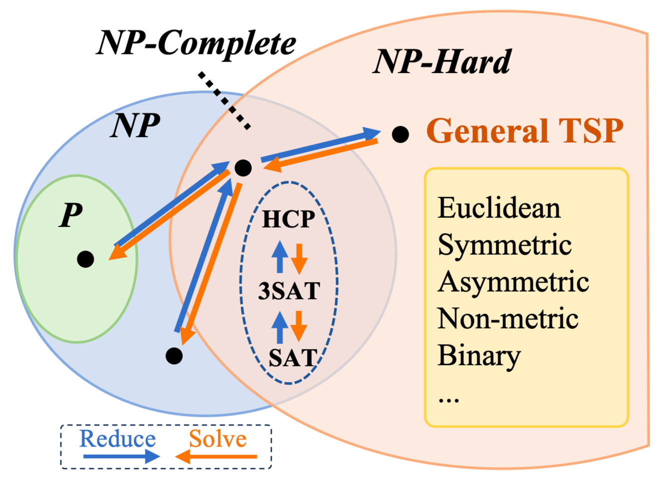
Paper   Code

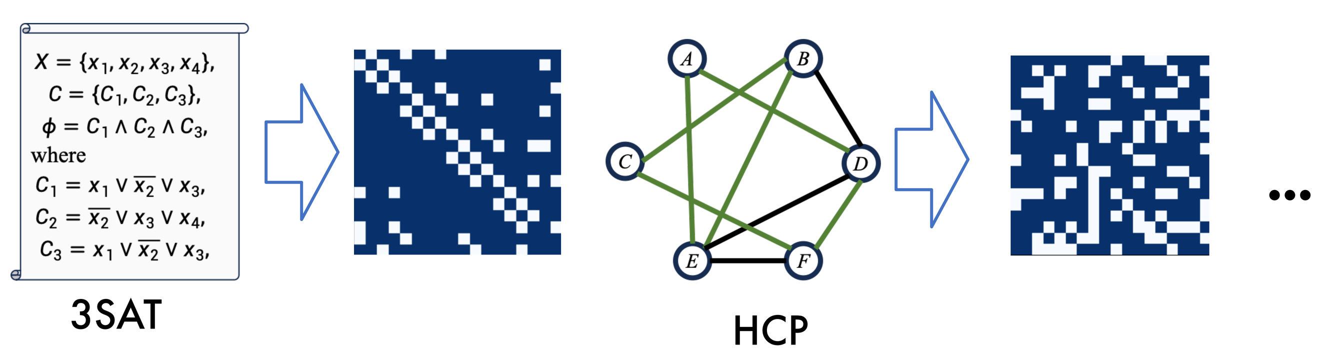
Unified Representation through Problem Reduction to General TSP

Let $\boldsymbol{x} \in \{0, 1\}^N$ denote the optimization variable. The feasible set Ω consists of $\boldsymbol{x}$ satisfying specific constraints as feasible solutions. A combinatorial optimization problem on graph G aims to find a feasible $\boldsymbol{x}$ that minimize the given objective function:

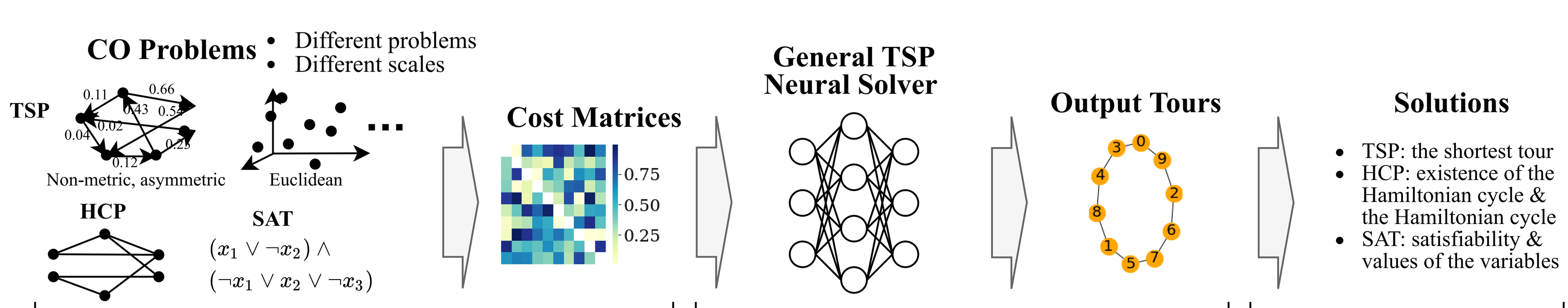
$$\min_{\boldsymbol{x}\in\{0,1\}^N} f(\boldsymbol{x}; G) \quad s.t. \quad \boldsymbol{x} \in \Omega$$



Various neural solvers have been devised for combinatorial optimization (CO), which are often tailored for specific problem types, e.g. TSP, HCP and SAT, etc. Yet, it remains an open question **how to achieve universality regarding problem representing and learning with a general framework**.



Unified Learning Framework for Matrix-Encoded General TSP



a) Problem reduction to general TSP   b) Problem solving   c) Result transformation

- We conceptualize **UniCO**, namely Unified Combinatorial Optimization learning framework, leveraging the rich expressivity of general TSP with arbitrary positive-valued matrix for unified representation of multiple CO problems (where reducible). We also construct standard datasets benchmarking the under-explored capacity of the general TSP world accordingly.
- We propose **MatPOENet**, namely Matrix encoding Network with Pseudo One-hot Embedding, a reinforced Transformer-based model which utilizes a novel size-agnostic node embedding to aid instance input, thereby significantly improving model scalability and performance of general TSP.
- We propose **MatDIFFNet**, namely Matrix encoding Diffusion Network, a supervised diffusion-based model which leverages a novel mix-noised reference map module, thus extending the promising ability of generative model for Euclidean TSP solving to matrix-formulated general TSP.
- We instantiate UniCO with the above two proposed neural backbones and one more existing method, and conduct **experiments on general TSP with four types of CO problem distributions, i.e., ATSP, 2DTSP, DHCP, and 3SAT**. Experiments show that measuring either the average TSP tour length or the average rate that solvers find optimal solutions for decisive tasks.

Overview: To instantiate the UniCO framework, we propose two models **1) MatPOENet (Graph Transformer + RL)**, improved upon MatNet to adapt to arbitrary-size TSP via our designed Pseudo One-hot Embedding (POE) as initial node feature with positional information; and **2) MatDIFFNet (Graph Diffusion + SL)**, leveraging the promising diffusion modeling for CO solving and combining distance matrix with noised solution to tackle ATSP.

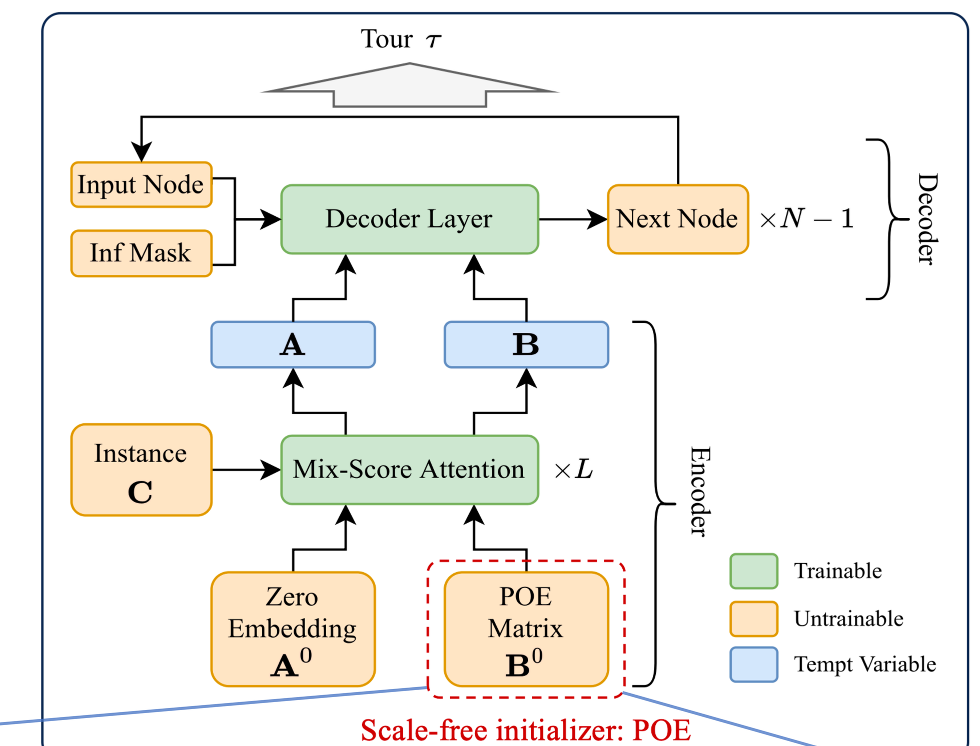
UniCO-MatPOENet

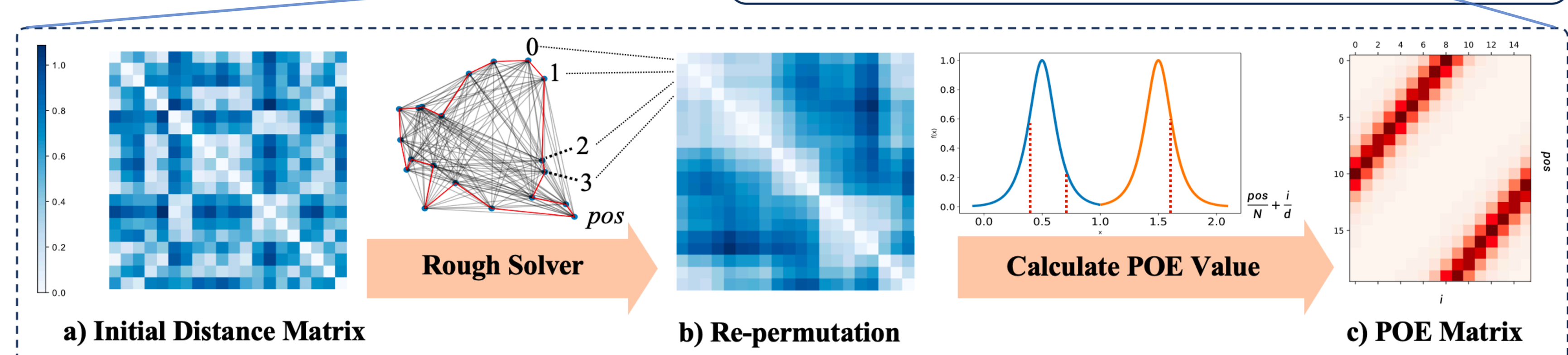
Reinforcement Learning:

$$\nabla_\theta J(\theta) \approx \frac{1}{N}\sum_{n=1}^{N}\left(L(\tau^n) - b(\mathbf{C})\right)\nabla_\theta \log p_\theta(\tau^n|\mathbf{C})$$

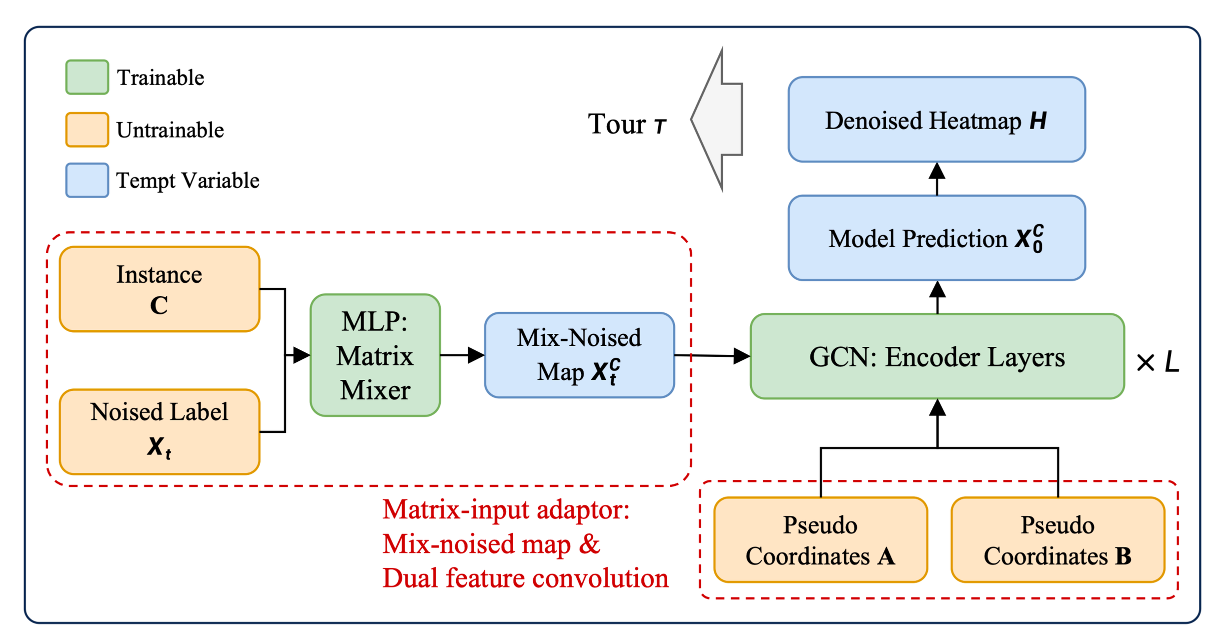
Pseudo One-hot Embedding:

$$\mathbf{P}_{pos,i} = \begin{cases} f\left(\frac{pos}{N} + \frac{i}{d} - \frac{1}{2}\right) & \text{if } \frac{pos}{N} + \frac{i}{d} \le 1 \\ f\left(\frac{pos}{N} + \frac{i}{d} - \frac{3}{2}\right) & \text{if } \frac{pos}{N} + \frac{i}{d} > 1 \end{cases}.$$





UniCO-MatDIFFNet



Soft Solution:

$$\mathbf{x}_t \in [0, 1]^{N\times 2}$$

Transition Matrix:

$$\mathbf{Q}_t = \begin{bmatrix} \beta_t & 1-\beta_t \\ 1-\beta_t & \beta_t \end{bmatrix}$$

The noising process: $q(\mathbf{x}_{1:T}|\mathbf{x}_0) = \prod_{t=1}^{T} q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \prod_{t=1}^{T} \mathrm{Cat}(\mathbf{x}_t; \mathbf{p} = \mathbf{x}_{t-1}\mathbf{Q}_t)$

The denoising process: $p_\theta(\mathbf{x}_{0:T}|G) = p(\mathbf{x}_T)\prod_{t=1}^{T} p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t, G)$

Mix-noised reference map: $\mathbf{x}_t^{\mathbf{C}} = W_{\text{mix2}}\left(\text{ReLU}\left(W_{\text{mix1}}(M)\right)\right)$

Dual feature updates for ATSP:

$$x_{A,i}^{l+1} = x_{A,i}^{l} + \text{ReLU}(\text{BN}(W_{A,1}^{l}x_{A,i}^{l} + \sum_{j\sim i} G_{ij}^{l} \odot (W_{A,2}^{l}x_{A,j}^{l} + W_{B,2}^{l}x_{B,j}^{l}))),$$

$$x_{B,i}^{l+1} = x_{B,i}^{l} + \text{ReLU}(\text{BN}(W_{B,1}^{l}x_{B,i}^{l} + \sum_{j\sim i} G_{ij}^{l} \odot (W_{A,2}^{l}x_{A,j}^{l} + W_{B,2}^{l}x_{B,j}^{l})^{\top})),$$

$$e_{ij}^{l+1} = e_{ij}^{l} + \text{ReLU}(\text{BN}(W_3^{l}e_{ij}^{l} + W_{A,4}^{l}x_{A,i}^{l} + W_{B,4}^{l}x_{B,j}^{l})) + W_5^{l}(\text{ReLU}(t^0)),$$

$$G_{A,ij}^{l} = \frac{\sigma(e_{ij}^{l})}{\sum_{j'\sim i}\sigma(e_{ij'}^{l}) + \epsilon},\ G_{B,ij}^{l} = \frac{\sigma((e_{ij}^{l})^{\top})}{\sum_{j'\sim i}\sigma((e_{ij'}^{l})^{\top}) + \epsilon},$$

Experiments

a. Overall Performance

Table 2: Main experimental results. Reported data for ATSP and 2DTSP are tour length. "Single": models trained and tested on each problem respectively. "Mixed": unified models trained with a mixture of 4 tasks on each scale. Asterisked (*): a unified model trained with a mixture of 4 tasks and 3 scales. **Bold**: the best result of neural solvers. Underlined: the reference results for computing the optimality gap. Red / blue boxes: ours that outperform LKH with 10K/500 trials respectively. Time: the average time (seconds) per instance solving over each line, with batch size set to 1.

Scale	Methods	Train Data	ATSP↓	2DTSP↓	DHCP (L↓, FR↑)		3SAT (L↓, FR↑)		Avg. L↓	Avg. Gap↓	Avg. FR↑	Time
Scale: $N \approx 20$	Gurobi	-	1.5349	3.8347	0.0000	100.00%	0.0000	100.00%	1.3424	-	100.00%	0.135
	LKH (10000)	-	1.5349	3.8347	0.0008	99.92%	0.0000	100.00%	1.3426	0.01%	99.96%	0.327
	LKH (500)	-	1.5349	3.8347	0.0056	99.44%	0.0000	100.00%	1.3438	0.11%	99.72%	0.038
	Nearest Neighbor	-	2.0069	4.5021	3.8556	0.48%	3.0504	0.32%	3.3428	149.02%	0.40%	0.000
	Farthest Insertion	-	1.7070	3.9695	3.3136	1.76%	4.8816	0.00%	3.4679	158.34%	0.88%	0.000
	MatNet	ATSP	1.5871	4.2612	2.9608	1.12%	3.4772	0.56%	3.0716	128.82%	0.84%	0.005
	MatNet	Mixed	1.6359	3.9114	0.9740	27.60%	3.4656	11.04%	2.4967	85.99%	19.32%	0.005
	MatNet-8x	Mixed	1.5645	3.8478	0.1936	80.92%	1.6272	1.36%	1.8083	34.71%	41.14%	0.037
	DIMES	Mixed	2.2335	4.1696	2.9448	2.67%	2.6660	2.12%	3.0035	123.74%	2.39%	0.035
	DIMES-AS(100)	Mixed	1.6790	3.9092	0.4596	60.12%	0.2828	77.12%	1.5826	17.90%	68.62%	0.522
	MatPOENet	Mixed	1.6445	3.8643	0.8676	32.60%	0.4540	61.88%	1.7076	27.21%	47.24%	0.006
	MatPOENet-8x	Mixed	1.5695	3.8389	0.1760	82.68%	0.0112	98.88%	1.3989	4.21%	90.78%	0.043
	MatPOENet*-8x	Mixed	**1.5506**	**3.8372**	**0.0556**	**94.44%**	**0.0008**	**99.92%**	**1.3610**	**1.39%**	**97.18%**	0.043
Scale: $N \approx 50$	Gurobi	-	1.5545	5.6952	0.0000	100.00%	0.0000	100.00%	1.8124	-	100.00%	0.296
	LKH (10000)	-	1.5548	5.6953	0.0000	100.00%	0.2784	74.80%	1.8821	3.85%	87.40%	0.513
	LKH (500)	-	1.5557	5.6964	0.0000	100.00%	0.4796	61.80%	1.9329	6.65%	80.90%	0.059
	Nearest Neighbor	-	2.0945	6.9977	5.1120	0.00%	5.9872	0.00%	5.0548	178.90%	0.00%	0.000
	Farthest Insertion	-	1.8387	6.0998	4.0224	5.28%	10.3964	0.00%	5.5893	208.39%	2.64%	0.001
	MatNet	ATSP	1.5753	7.3618	1.4856	11.80%	8.4020	0.00%	4.7062	159.67%	5.90%	0.007
	MatNet	Mixed	1.8098	6.0000	0.9288	30.84%	1.1900	30.52%	2.4821	36.95%	30.68%	0.007
	MatNet-8x	Mixed	1.7340	5.8664	0.3056	71.52%	0.2992	73.08%	2.0513	13.18%	72.30%	0.064
	GLOP	Single	1.8885	6.6499	3.7244	0.84%	4.9816	0.76%	4.3111	137.87%	0.80%	0.115
	DIMES	Mixed	2.3341	6.6271	3.1788	1.56%	5.3656	0.12%	4.3764	141.47%	0.84%	0.055
	DIMES-AS(100)	Mixed	1.6920	5.9447	0.5908	46.04%	1.5830	20.44%	2.4528	35.33%	33.24%	2.016
	MatPOENet-8x	Single	**1.5643**	**5.7042**	0.0652	93.52%	0.1888	81.72%	**1.8806**	**3.76%**	87.62%	0.066
	MatPOENet	Mixed	1.6881	5.7694	0.1444	86.20%	1.3644	27.08%	2.2416	23.68%	56.64%	0.009
	MatPOENet-8x	Mixed	1.6417	5.7283	**0.0172**	**98.28%**	0.2456	77.60%	1.9082	5.29%	87.94%	0.067
	MatPOENet*-8x	Mixed	1.6285	5.7575	0.0280	97.20%	0.1172	88.44%	1.8828	3.88%	**92.82%**	0.067
	MatDIFFNet	Single	2.0713	5.7954	2.0992	15.32%	0.0464	98.16%	2.5031	38.11%	56.74%	0.157
	MatDIFFNet-2OPT	Single	1.7186	5.7279	0.8324	44.08%	**0.0188**	**98.64%**	2.0744	14.46%	71.36%	0.165
	MatDIFFNet	Mixed	1.8385	6.2332	2.0648	15.76%	0.1112	94.68%	2.5619	41.35%	55.22%	0.155
	MatDIFFNet-2OPT	Mixed	1.6591	5.8619	0.8192	44.52%	0.0496	95.64%	2.0975	15.73%	70.08%	0.164
Scale: $N \approx 100$	Gurobi	-	1.5661	7.7619	0.0000	100.00%	0.0000	100.00%	2.3320	-	100.00%	0.689
	LKH (10000)	-	1.5674	7.7709	0.0000	100.00%	1.0008	44.80%	2.5848	10.84%	72.40%	0.811
	LKH (500)	-	1.5704	7.8015	0.0000	100.00%	1.6656	28.08%	2.7594	18.33%	64.04%	0.095
	Nearest Neighbor	-	2.1321	9.6696	5.4016	0.20%	8.3236	0.00%	6.3859	173.84%	0.10%	0.002
	Farthest Insertion	-	1.9333	8.4847	3.1256	26.64%	23.5160	0.00%	9.2649	297.29%	13.32%	0.003
	MatNet	ATSP	**1.6217**	19.0644	17.8620	0.00%	40.1188	0.00%	19.6667	743.34%	0.00%	0.015
	MatNet	Mixed	1.9849	8.2551	0.9776	31.68%	2.0408	13.84%	3.3146	42.14%	22.76%	0.018
	MatNet-8x	Mixed	1.9210	8.1028	0.3640	69.60%	0.7740	50.76%	2.7904	19.66%	60.18%	0.095
	GLOP	Single	1.8491	8.8849	2.7850	2.00%	6.4280	0.08%	4.9868	113.84%	1.04%	0.176
	DIMES	Mixed	2.5186	9.5777	3.8064	1.16%	3.8064	0.00%	6.4018	174.52%	0.58%	0.124
	DIEMS-AS(100)	Mixed	1.6968	8.3390	0.8480	24.00%	2.8040	7.16%	3.4220	46.74%	15.58%	8.437
	MatPOENet	Mixed	1.9183	8.2987	0.0984	90.28%	1.0704	32.32%	2.8465	22.06%	61.30%	0.017
	MatPOENet-8x	Mixed	1.8655	8.1719	0.0052	99.48%	0.2440	77.12%	2.5717	10.28%	**88.30%**	0.094
	MatPOENet*-8x	Mixed	1.7607	8.0817	**0.0012**	**99.88%**	0.3244	70.92%	**2.5420**	**9.01%**	85.40%	0.095
	MatDIFFNet	Single	1.9432	7.9684	4.4536	2.96%	0.0404	98.44%	3.6014	54.43%	50.70%	0.103
	MatDIFFNet-2OPT	Single	1.7165	**7.8482**	1.1404	37.72%	**0.0240**	**98.60%**	2.6823	15.02%	68.16%	0.112
	MatDIFFNet	Mixed	1.8763	8.9030	3.2524	5.68%	0.1940	90.52%	3.5564	52.50%	48.10%	0.102
	MatDIFFNet-2OPT	Mixed	1.6965	8.1804	0.9148	43.04%	0.0952	91.44%	2.7217	16.71%	67.24%	0.114

Table 3: Results of both solving time and solving quality comparing Mat-X-Net (ours) and different settings of LKH. LKH-N: LKH with 1 *runs* and N *max_trials*. Batch size = 1.

Scale	Method	Time↓	ATSP↓	2DTSP↓	DHCP (L↓, FR↑)		3SAT (L↓, FR↑)		Avg. L↓
$N \approx 50$	MatPOENet	7m31s	1.6417	5.7283	0.0172	98.28%	0.2456	77.60%	1.9082
	MatDIFFNet	21m48s	1.7186	5.7279	0.8324	44.08%	0.0188	98.64%	2.0744
	LKH-500	9m9s	1.5557	5.6964	0.0000	100.00%	0.4796	61.80%	1.9329
	LKH-1000	13m53s	1.5554	5.6957	0.0000	100.00%	0.4160	65.68%	1.9168
	LKH-10000	1h22m	1.5548	5.6953	0.0000	100.00%	0.2784	74.80%	1.8821
$N \approx 100$	MatPOENet	15m35s	1.8655	8.1719	0.0052	99.48%	0.2440	77.12%	2.5717
	MatDIFFNet	28m21s	1.7165	7.8482	1.1404	37.72%	0.0240	98.60%	2.6823
	LKH-500	15m49s	1.5704	7.8015	0.0000	100.00%	1.6656	28.08%	2.7594
	LKH-1000	24m39s	1.5692	7.7909	0.0000	100.00%	1.4400	32.52%	2.7000
	LKH-10000	2h15m	1.5674	7.7709	0.0000	100.00%	1.0008	44.80%	2.5848

←b. Efficiency & Quality v.s. LKH

↓c. Cross-scale/task Fine-tuning Results

Table 13: Results of the cross-scale finetuning experiments on $N \approx 100$ sets. The MatPOENet model is pretrained under UniCO framework with different dataset of $N \approx 50$ for 2,000 epochs and subsequently finetuned on mixed data of $N \approx 100$ scale for (a much fewer) 500 iterations.

Pretrain data	Finetune data	ATSP↓	2DTSP↓	DHCP (L↓, FR↑)		3SAT (L↓, FR↑)		**Avg. L↓**
Mixed-50	-	2.5656	8.5404	23.5064	0.00%	17.5564	0.00%	13.0422
Mixed-50	Mixed-100	1.9798	**8.0573**	1.7796	6.60%	2.0664	11.68%	3.4708
ATSP-50	Mixed-100	**1.8855**	8.3838	**0.6712**	**46.72%**	0.2888	72.76%	**2.8073**
Mixed-100	-	1.8655	8.1719	0.0052	99.48%	**0.2440**	**77.12%**	2.5717

Table 12: Results of the cross-task finetuning on 3SAT. MatPOENet is pretrained under UniCO framework with dataset comprising ATSP, 2DTSP and DHCP instances of $N \approx 50$ for 2,000 epochs and subsequently finetuned on the new task of 3SAT data for (a much fewer) 500 iterations.

Description	3SAT (L)↓	3SAT(FR)↑	#Epochs
Pretrained on ATSP, 2DTSP, DHCP w/o Finetuning	1.4080	17.92%	2000
Pretrained on ATSP, 2DTSP, DHCP w/ Finetuning on 3SAT	0.0404	95.96%	50
	0.0360	96.40%	100
	0.0292	97.08%	200
Trained on merely 3SAT (control group)	0.0400	96.08%	2000