Learning to Solve the Quadratic Assignment Problem with Warm-Started MCMC Finetuning

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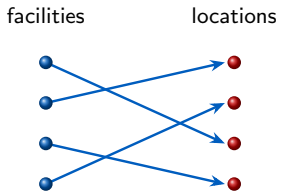
Outline

Quadratic Assignment Problem (QAP)

- A QAP instance is specified by a flow matrix $\boldsymbol{F} = (F_{ij})$ and a distance matrix $\boldsymbol{D} = (D_{kl})$.
- A permutation $\pi \in \Pi_n$ assigns each facility to one location.
- We use the permutation formulation:

$$\min_{\pi \in \Pi_n} \quad f(\pi; \mathcal{P}) := \sum_{i=1}^{n} \sum_{j=1}^{n} F_{ij}\, D_{\pi(i)\pi(j)}.$$



π maps facilities to locations

Equivalent matrix form

$$f(\pi; \mathcal{P}) = \langle \boldsymbol{F}, \boldsymbol{X}_\pi \boldsymbol{D} \boldsymbol{X}_\pi^\top \rangle, \qquad \boldsymbol{X}_\pi \mathbf{1} = \boldsymbol{X}_\pi^\top \mathbf{1} = \mathbf{1}.$$

Here $\boldsymbol{X}_\pi$ is the permutation matrix induced by π.

Why is QAP difficult?

- Broad modeling power: facility layout, keyboard design, graph matching, graph partitioning, TSP reductions, and bandwidth minimization.
- Severe computational barrier: QAP is NP-hard and NP-hard to approximate; exact methods are often limited beyond $n \approx 20$.
- Strong heuristics exist, e.g., simulated annealing, tabu search, and memetic algorithms, but their performance is instance-dependent.
- Learning is attractive: reuse structure across instances and exploit GPU parallelism.
- The key challenge is that a QAP instance contains two coupled graphs, not a single graph.

Need a solver that keeps the speed of learned priors while adapting to unseen instance structures.

Brief literature review

- **Traditional QAP heuristics**
  - Ro-TS [Taillard 1991] and BMA [Benlic et al. 2015] are highly competitive baselines.
  - Robustness can degrade on hard structured families such as Taixxeyy [Drezner et al. 2005].
- **Learning-based QAP / graph matching**
  - Association-graph models use n^2 pair nodes [Wang et al. 2021; Liu et al. 2023].
  - Solution-aware Transformer learns swap improvement, but assumes complete initial solutions [Tan et al. 2024].
- **Deployment-time refinement**
  - Active search finetunes at test time [Bello et al. 2016; Hottung et al. 2022; Qiu et al. 2022].
  - Auto-regressive solvers restart construction after each update; prior high-quality solutions are hard to reuse.

Outline

Probabilistic learning formulation

- Replace direct search over Π_n by an optimization over distributions:

$$\min_{p \in \Delta(\Pi_n)} \mathbb{E}_{\pi \sim p} \left[f(\pi; \mathcal{P}) \right].$$

- This is equivalent to the deterministic QAP:

optimal probability distributions are supported on optimal permutations.

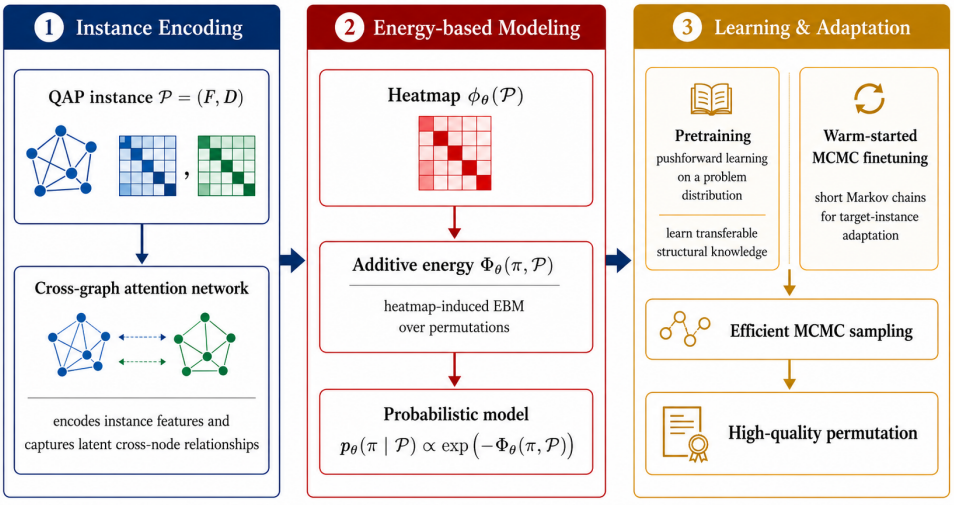
- Use an instance-conditioned model $p_\theta(\cdot \mid \mathcal{P})$ and learn over a distribution of instances Γ:

$$\min_{\theta} \mathbb{E}_{\mathcal{P} \sim \Gamma} \mathbb{E}_{\pi \sim p_\theta(\cdot|\mathcal{P})} \left[f(\pi; \mathcal{P}) \right].$$

- To smooth the rugged landscape, apply a 2-swap local improvement map $\mathcal{T} : \Pi_n \to \Pi_n$:

$$\begin{aligned} \min_{\theta \in \mathbb{R}^d} \quad \mathcal{L}(\theta) &:= \mathbb{E}_{\mathcal{P} \sim \Gamma} \mathbb{E}_{\sigma \sim \mathcal{T}_\sharp p_\theta(\cdot|\mathcal{P})} \left[f(\sigma; \mathcal{P}) \right] \\ &= \mathbb{E}_{\mathcal{P} \sim \Gamma} \mathbb{E}_{\pi \sim p_\theta(\cdot|\mathcal{P})} \left[f(\mathcal{T}(\pi); \mathcal{P}) \right]. \end{aligned}$$

PLMA framework at a glance



Energy-based model over permutations

- Given a heatmap $\phi(\theta, \mathcal{P}) \in \mathbb{R}^{n \times n}$:

$$p_\theta(\pi \mid \mathcal{P}) \propto \exp(\langle \boldsymbol{X}_\pi, \phi \rangle) = \exp(\Phi_\theta(\pi)) .$$

- Additive score:

$$\Phi_\theta(\pi) = \sum_{i=1}^{n} \phi_{i,\pi(i)}.$$

- For a symmetric 2-swap proposal (a, b):

$$\frac{p_\theta(\pi')}{p_\theta(\pi)} = \exp\left(\phi_{a,\pi(b)} + \phi_{b,\pi(a)} - \phi_{a,\pi(a)} - \phi_{b,\pi(b)}\right) .$$

- Each MH acceptance step has $O(1)$ score-update cost.

Why this formulation?

- Directly samples feasible permutations.
- Additivity makes swap proposals cheap.
- Warm-started MCMC naturally refines previous high-quality solutions.

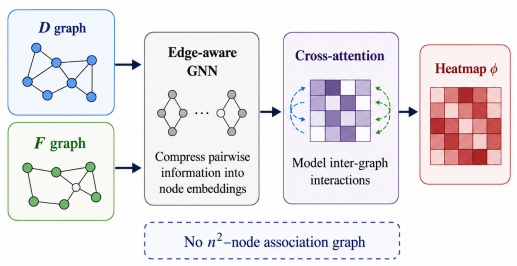
Cross-graph attention network

- A QAP instance is represented as two weighted graphs: location graph $\boldsymbol{D}$ and facility graph $\boldsymbol{F}$.
- Edge-aware GNN layers compress pairwise information into node embeddings:

$$\boldsymbol{D}, \boldsymbol{F} \quad \Longrightarrow \quad \boldsymbol{H}_D, \boldsymbol{H}_F \in \mathbb{R}^{n \times d}.$$

- Cross-attention fills the missing interactions between the two disconnected graphs.
- A dot product followed by log-Sinkhorn produces the heatmap:

$$\phi_\theta(\mathcal{P}) \;=\; \text{log-Sinkhorn}\left(C \tanh\left(\frac{\boldsymbol{H}_F \boldsymbol{H}_D^{\mathrm{T}}}{\sqrt{d}} \right) \right).$$



Scalability

The node space remains $O(2n)$, avoiding an $O(n^2)$ association graph while still modeling inter-graph coupling.

Stage I: pretraining with pushforward transformation

- Goal: learn transferable structural priors from a training distribution Γ.
- At each step:
  1. sample a batch $\{\mathcal{P}_i\}_{i=1}^{B} \sim \Gamma$;
  2. draw N permutations by parallel MH chains;
  3. refine each sample by $\hat{\pi}_{i,k} = \mathcal{T}(\pi_{i,k})$;
  4. update θ using the improved costs $f(\hat{\pi}_{i,k}; \mathcal{P}_i)$.
- The gradient estimator uses an instance-wise baseline:

$$\hat{G} = \frac{1}{B(N-1)} \sum_{i=1}^{B} \sum_{k=1}^{N} \left(\hat{f}_{i,k} - b_i \right) \nabla_\theta \Phi_\theta(\pi_{i,k}), \qquad b_i = \frac{1}{N} \sum_{k=1}^{N} \hat{f}_{i,k}.$$

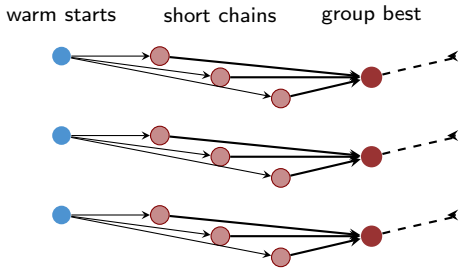
- Long chains are used here to stabilize sampling in the cold-start regime.

Stage II: batch-wise warm-started MCMC finetuning

- Start from the pretrained EBM and target instances $\{\mathcal{P}_i\}_{i=1}^{B}$.
- Generate K high-quality initial states with long-run MH sampling.
- For each state, launch M short chains:

$$\pi_{i,k} \quad \Longrightarrow \quad \{\pi_{i,k}^{m}\}_{m=1}^{M} \quad \Longrightarrow \quad \{\mathcal{T}(\pi_{i,k}^{m})\}_{m=1}^{M}.$$

- Update the shared model with one batch gradient over all instances and chains.
- Retain the best sample within each group k as the next warm start.



preserve quality while keeping diversity

Design principle

Short chains keep exploration near promising regions already discovered by the previous iteration.

Outline

Experimental setup

- **Hardware:** NVIDIA Tesla A800 GPUs and Intel Xeon Gold 6326 CPUs.
- **Datasets:**
  - synthetic QAP: geometrically structured instances, $n \in \{20, 50, 100\}$;
  - out-of-distribution large-scale random instances, $n \in \{200, 500\}$;
  - QAPLIB and Taixxeyy benchmarks.
- **Baselines:** Ro-TS, BMA, Connolly's SA, IPFP, SM, RRWM, NGM, SAWT.
- **Metrics:** average objective, relative gap, total runtime; for Taixxeyy, mean and range over 10 independent runs.

Synthetic QAP results

	QAP20			QAP50			QAP100		
Algorithm	Cost	Gap	Time	Cost	Gap	Time	Cost	Gap	Time
Ro-TS (1k)	54.38	0.01%	17.04s	375.99	0.14%	4m35s	1593.27	0.13%	38m56s
Ro-TS (5k)	**54.37**	**0.00%**	1m25s	**375.48**	**0.00%**	22m53s	1591.25	0.00%	3h15m
BMA	**54.37**	**0.00%**	1m57s	375.60	0.03%	15m53s	1591.58	0.02%	2h21m
C-SA	54.53	0.28%	1m57s	376.56	0.29%	21m32s	1592.95	0.11%	2h45m
IPFP	55.11	1.37%	2.04s	378.76	0.88%	11.47s	1600.27	0.57%	1m34s
IPFP (10)	54.54	0.31%	20.97s	376.60	0.30%	2m30s	1594.76	0.22%	17m34s
RRWM	71.30	31.09%	11.30s	428.78	14.14%	39.23s	1700.33	6.86%	6m32s
SM	64.38	18.45%	0.22s	426.92	13.70%	7.14s	1753.10	10.17%	1m40s
NGM	62.93	15.87%	24.78s	429.69	14.46%	1m16s	1773.71	11.47%	2m29s
SAWT (10k)	54.72	0.64%	3m41s	380.92	1.45%	5m36s	1617.30	1.64%	10m43s
PLMA ($T = 1$)	54.63	0.48%	0.06s	379.79	1.15%	0.41s	1607.84	1.04%	4.27s
PLMA ($T = 50$)	**54.37**	**0.00%**	2.57s	375.55	0.20%	19.88s	1591.73	0.03%	3m30s
PLMA ($T = 200$)	**54.37**	**0.00%**	9.36s	**375.48**	**0.00%**	1m19s	**1591.23**	**0.00%**	13m58s

- The pretrained model already provides strong zero-shot solutions.
- Finetuning quickly closes the remaining gap while retaining a large runtime advantage.

Large-scale QAP results

	QAP200		QAP500	
Algorithm	Gap	Time	Gap	Time
Ro-TS	0.00%	3h48m	0.00%	29h59m
BMA	0.01%	2h58m	-0.09%	23h16m
SAWT (10k)	1.44%	8m33s	1.55%	48m36s
PLMA ($T = 1$)	0.53%	7.50s	0.38%	1m31s
PLMA ($T = 50$)	**-0.01%**	6m15s	**-0.12%**	1h15m

PLMA remains competitive or better than strong handcrafted baselines at $n = 200, 500$, with substantially lower runtime.

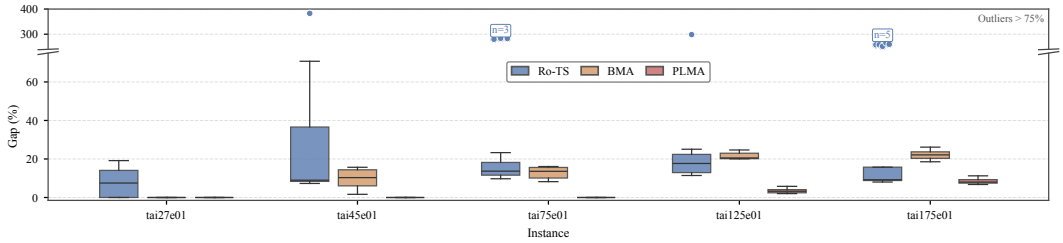
QAPLIB benchmark

	Ro-TS		BMA		SAWT		IPFP		PLMA	
Class	Gap	Time	Gap	Time	Gap	Time	Gap	Time	Gap	Time
bur (26)	**0.00%**	0.12	**0.00%**	0.03	3.95%	14.67	0.05%	0.33	**0.00%**	0.08
chr (12-25)	0.48%	0.16	0.18%	0.14	147.54%	14.18	14.90%	0.26	**0.00%**	0.31
els (19)	**0.00%**	0.02	**0.00%**	0.02	47.37%	14.24	10.18%	0.36	**0.00%**	0.09
esc (16-128)	**0.00%**	0.62	**0.00%**	0.01	43.29%	15.07	0.39%	0.63	**0.00%**	0.07
had (12-20)	**0.00%**	0.00	**0.00%**	0.00	5.17%	14.23	0.08%	0.39	**0.00%**	0.05
kra (30-32)	**0.00%**	0.24	**0.00%**	0.07	32.92%	14.77	0.65%	0.62	**0.00%**	0.31
lipa (20-90)	0.03%	3.28	**0.02%**	2.35	1.40%	17.32	1.07%	4.93	0.08%	1.57
nug (12-30)	**0.00%**	0.02	**0.00%**	0.02	19.25%	14.39	0.05%	0.38	**0.00%**	0.17
rou (12-20)	**0.00%**	0.04	**0.00%**	0.04	15.09%	14.25	0.77%	0.33	**0.00%**	0.08
scr (12-20)	**0.00%**	0.01	**0.00%**	0.01	33.92%	14.22	1.24%	0.28	**0.00%**	0.08
sko (42-100)	0.05%	29.22	**0.03%**	21.00	16.17%	19.06	0.30%	8.40	**0.03%**	7.01
ste (36)	0.01%	0.53	**0.00%**	0.30	107.95%	14.95	1.81%	0.70	**0.00%**	0.55
tai (10-256)	0.23%	25.16	0.21%	19.06	34.67%	16.62	0.92%	3.33	**0.20%**	4.73
tho (30-150)	**0.04%**	38.74	**0.04%**	26.59	24.05%	17.19	0.42%	12.46	**0.04%**	6.42
wil (50-100)	**0.02%**	26.06	**0.02%**	18.41	9.52%	17.64	0.12%	9.66	**0.02%**	6.82
Average	0.11%	9.68	0.07%	7.06	37.82%	15.85	2.15%	2.73	**0.06%**	2.16

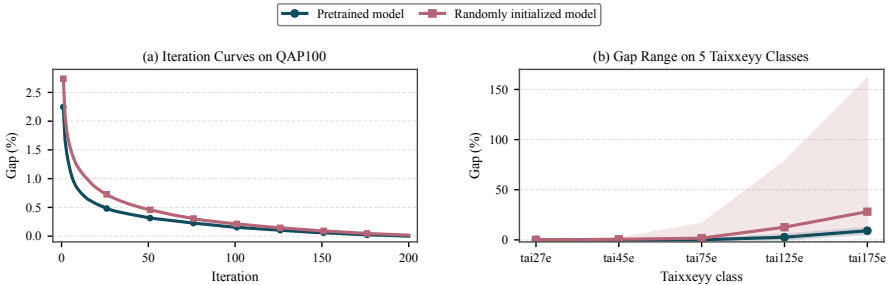
PLMA attains the lowest average gap and the shortest average time among the compared heuristic baselines.

Robustness on Taixxeyy instances

	Ro-TS			BMA			IPFP			PLMA		
Class	mean	[min,max]	time	mean	[min,max]	time	mean	[min,max]	time	mean	[min,max]	time
tai27e	41.50	[0.11,221.08]	0.57	0.12	[0.00,0.67]	0.18	19.47	[6.14,34.11]	0.38	**0.00**	**[0.00,0.00]**	0.08
tai45e	101.89	[1.00,400.60]	3.83	8.39	[0.74,17.63]	2.21	22.01	[8.26,36.98]	1.03	**0.00**	**[0.00,0.00]**	0.18
tai75e	111.28	[6.20,280.01]	18.49	15.41	[5.77,22.76]	11.21	27.64	[17.56,36.78]	2.52	**0.08**	**[0.00,0.63]**	1.27
tai125e	82.53	[7.65,265.54]	72.52	16.51	[10.56,21.72]	66.01	26.93	[20.64,32.67]	8.52	**3.65**	**[0.78,6.32]**	8.65
tai175e	67.86	[9.11,260.98]	158.18	21.07	[15.15,26.56]	193.65	23.32	[17.70,28.11]	16.86	**9.09**	**[5.96,12.24]**	14.43
Average	81.01	[4.82,285.64]	50.72	12.30	[6.44,17.87]	54.65	23.87	[14.06,33.73]	5.86	**2.56**	**[1.35,3.84]**	**4.92**



Ablation: why the two-stage design matters



- Pretrained finetuning reaches lower gaps in fewer iterations on in-distribution random QAP100.
- On Taixxeyy, pretraining reduces both mean gap and variability across hard instance classes.
- The warm-started short-chain stage can exploit the pretrained prior instead of restarting search from scratch.

Conclusions

- PLMA formulates QAP solving as learning an instance-conditioned distribution over permutations.
- The pushforward learning objective trains the sampler toward regions that become high-quality after local improvement.
- The additive EBM enables constant-time 2-swap MH score updates and naturally supports warm starts.
- Two-stage learning is central:
  - pretraining learns transferable structural priors;
  - deployment-time finetuning adapts through short warm-started MCMC chains.
- Experiments show strong performance on synthetic QAP, QAPLIB, Taixxeyy and large-scale instances.

Many Thanks For Your Attention!