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Scalable Optimal Transport in High Dimensions for Graph Distances, Embedding Alignment, and More

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Massively scalable optimal transport: Sparse and LCN-Sinkhorn

Entropy-regularized optimal transport

$$\bar{\boldsymbol{P}} = \arg\min_{\boldsymbol{P}} \langle \boldsymbol{P}, \boldsymbol{C} \rangle_{\mathrm{F}} - \lambda H(\boldsymbol{P})$$

Solvable via Sinkhorn algorithm (alternating matrix normalization):

$$\boldsymbol{K} = \mathrm{e}^{-\boldsymbol{C}/\lambda}$$

$$\boldsymbol{s}^{(i)} = \boldsymbol{p} \oslash (\boldsymbol{K}\boldsymbol{t}^{(i-1)}), \qquad \boldsymbol{t}^{(i)} = \boldsymbol{q} \oslash (\boldsymbol{K}^T \boldsymbol{s}^{(i)})$$

$$\bar{\boldsymbol{P}} = \mathrm{diag}(\bar{\boldsymbol{s}})\, \boldsymbol{K}\, \mathrm{diag}(\bar{\boldsymbol{t}})$$

Parallelizable, runs in $\mathcal{O}(n^2)$ → $\boldsymbol{K}$ already has that many entries!

Sparse Sinkhorn

$\boldsymbol{K}$ exponential in $\boldsymbol{C}$ → only near neighbors important!

Sparsely approximate $\boldsymbol{K}$:

$$K^{\mathrm{sp}}_{ij} = \begin{cases} K_{ij} & \text{if } x_i, x_j \text{ are near,} \\ 0 & \text{otherwise} \end{cases}$$

Calculate P via Sinkhorn algorithm: $\bar{\boldsymbol{P}} \approx \bar{\boldsymbol{P}}^{\mathrm{sp}} = \mathrm{diag}(\bar{\boldsymbol{s}})\, \boldsymbol{K}^{\mathrm{sp}}\, \mathrm{diag}(\bar{\boldsymbol{t}})$
Runs in $\mathcal{O}(n \log n)$!

Locally corrected Nyström (LCN)

How to incorporate *short- and long-range* interactions?

Correct low-rank Nyström approximation with sparse values:

$$\boldsymbol{K}_{\mathrm{Nys}} = \boldsymbol{U}\boldsymbol{A}^{-1}\boldsymbol{V}$$

$$\boldsymbol{K}_{\mathrm{LCN}} = \boldsymbol{K}_{\mathrm{Nys}} - \boldsymbol{K}^{\mathrm{sp}}_{\mathrm{Nys}} + \boldsymbol{K}^{\mathrm{sp}}$$

LCN is a general kernel approximation.
We can still use the Sinkhorn algorithm → LCN-Sinkhorn, runs in $\mathcal{O}(n \log n + nl^2)$

GTN: GNN with optimal transport -48% error for graph distance learning

Graph Transport Network (GTN)

Graph neural network (GNN) generates node embeddings
Embeddings matched using Sinkhorn

→ Learns graph distances via backpropagation

Varying numbers of nodes → **learnable unbalanced OT**
Bipartite matching (BP) matrix for optimal transport
(Scaled) norms as deletion cost

$$\boldsymbol{C}_{BP} = \begin{bmatrix} \boldsymbol{C} & \boldsymbol{C}^{(\mathbf{p},\varepsilon)} \\ \boldsymbol{C}^{(\varepsilon,\mathbf{q})} & \boldsymbol{C}^{(\varepsilon,\varepsilon)} \end{bmatrix}, \quad \boldsymbol{C}^{(\mathbf{p},\varepsilon)}_{ij} = \begin{cases} c_{i,\varepsilon} & i = j \\ 0 & i \neq j \end{cases}, \quad \boldsymbol{C}^{(\varepsilon,\mathbf{q})}_{ij} = \begin{cases} c_{\varepsilon,j} & i = j \\ 0 & i \neq j \end{cases}, \quad \boldsymbol{C}^{(\varepsilon,\varepsilon)}_{ij} = 0$$

Multi-head OT: OT with multiple embeddings & varying regularization λ

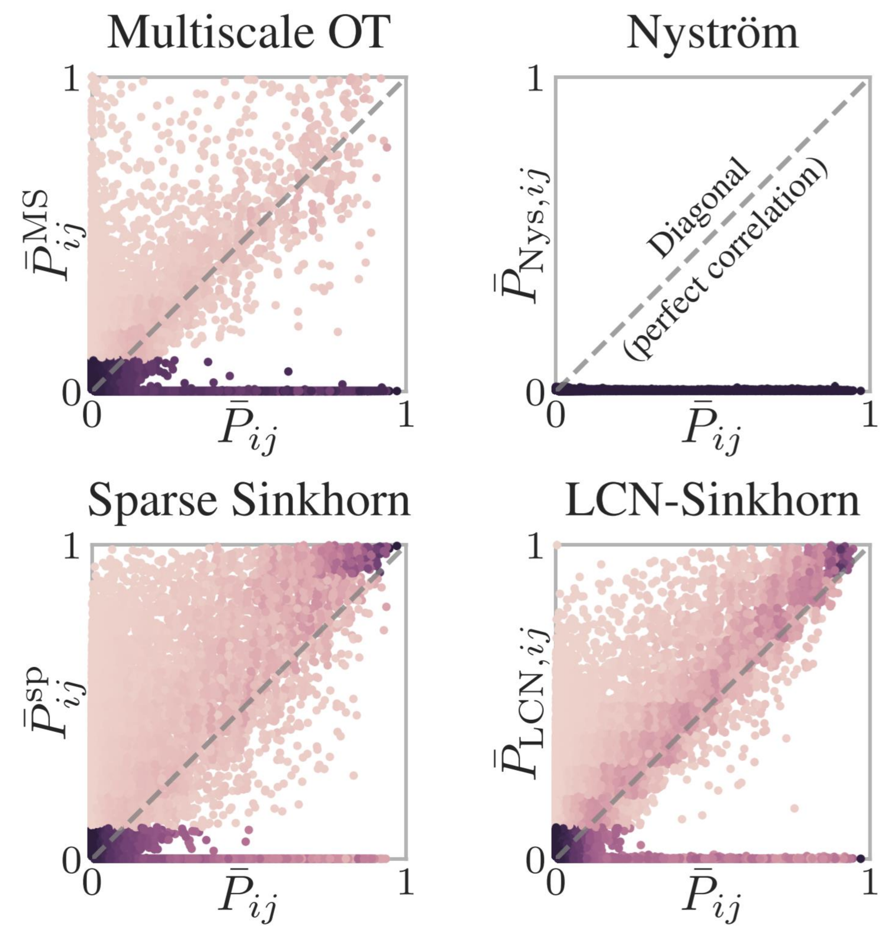
Model	Linux	AIDS30	Pref. att.
SiamMPNN	0.09	13.8	12.1
SimGNN	0.039	4.5	8.3
GMN	0.015	10.3	7.8
GTN, 1 head	0.022	3.7	4.5
8 OT heads	**0.012**	**3.2**	**3.5**
Balanced OT	0.034	15.3	27.4

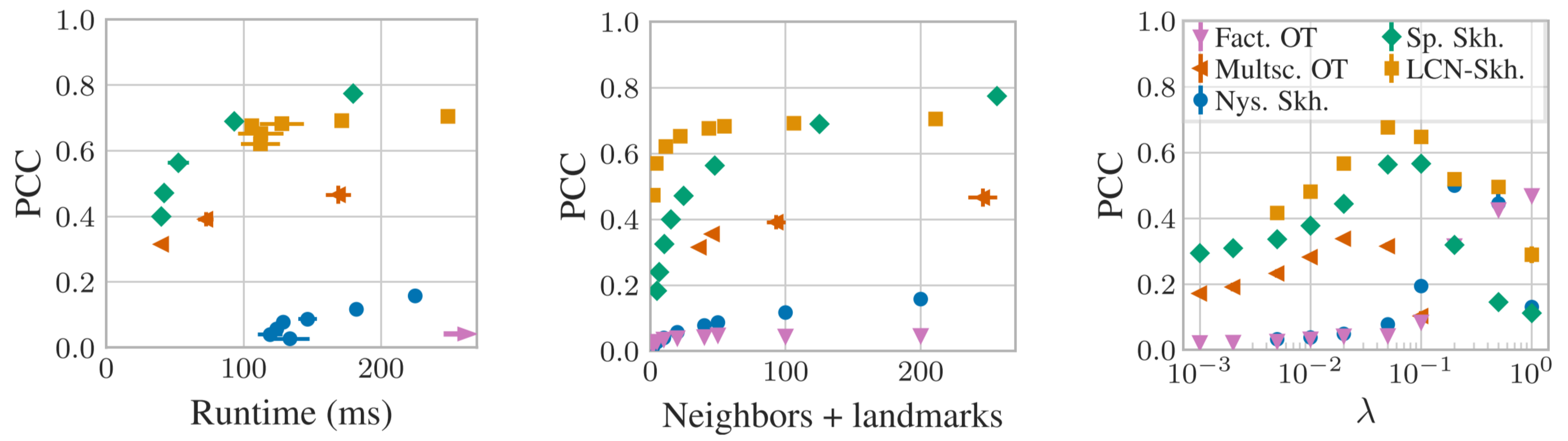
Method	AIDS 30	Pref. att.	Pref. att. 200
Full Sinkhorn	**3.7**	4.5	1.3
Nyström Skh.	**3.6**	6.2	2.4
Multiscale OT	11.2	27.4	6.7
Sparse Skh.	44	40.7	7.6
LCN-Sinkhorn	4.0	**5.1**	**1.4**

LCN: Provably better approximation, same convergence

- Sparse corrections provably reduce kernel approximation error of Nyström for uniform and clustered data [Theorem 1&2].
- Better kernel approximation directly translates to better Sinkhorn approximation [Theorem 3].
- Sparse and LCN-Sinkhorn converge in $\mathcal{O}(\ln \min \boldsymbol{K} / \varepsilon)$, like full Sinkhorn [Theorem 4].
- Sparse and LCN-Sinkhorn allow fast backpropagation via analytical gradients [Prop. 1].

Fast & accurate transport plan and embedding alignment





Embedding alignment

3x faster & 3.1pp more accurate

Method	Time (s)	Avg. accuracy
Original	268	67.9%
Full Sinkhorn	402	70.1%
Multiscale OT	88.2	26.8%
Nyström Sinkhorn	102	47.8%
Sparse Sinkhorn	**49.2**	68.4%
LCN-Sinkhorn	86.8	**71.0%**