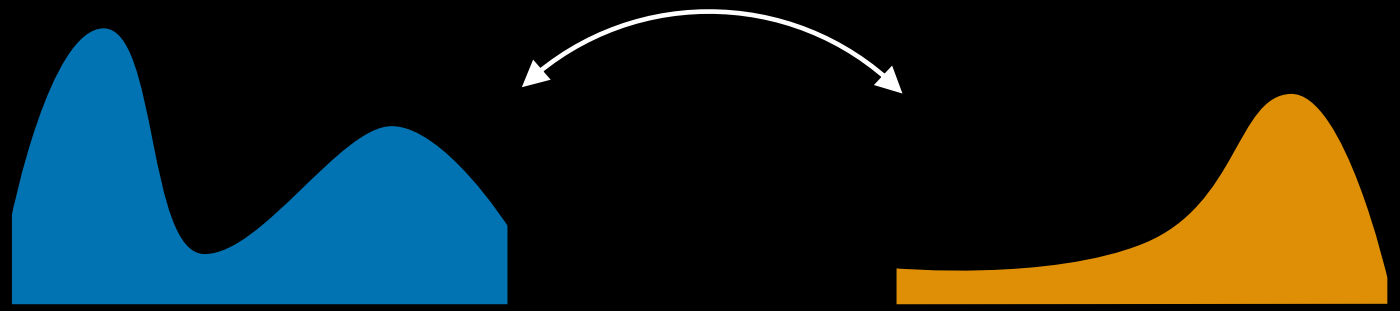
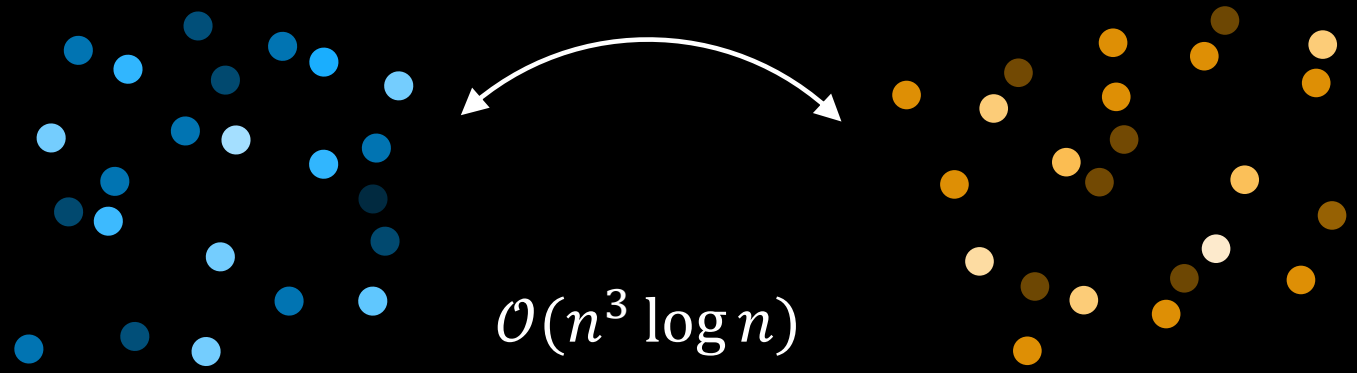
SCALABLE OPTIMAL TRANSPORT IN HIGH DIMENSIONS FOR GRAPH DISTANCES, EMBEDDING ALIGNMENT, AND MORE

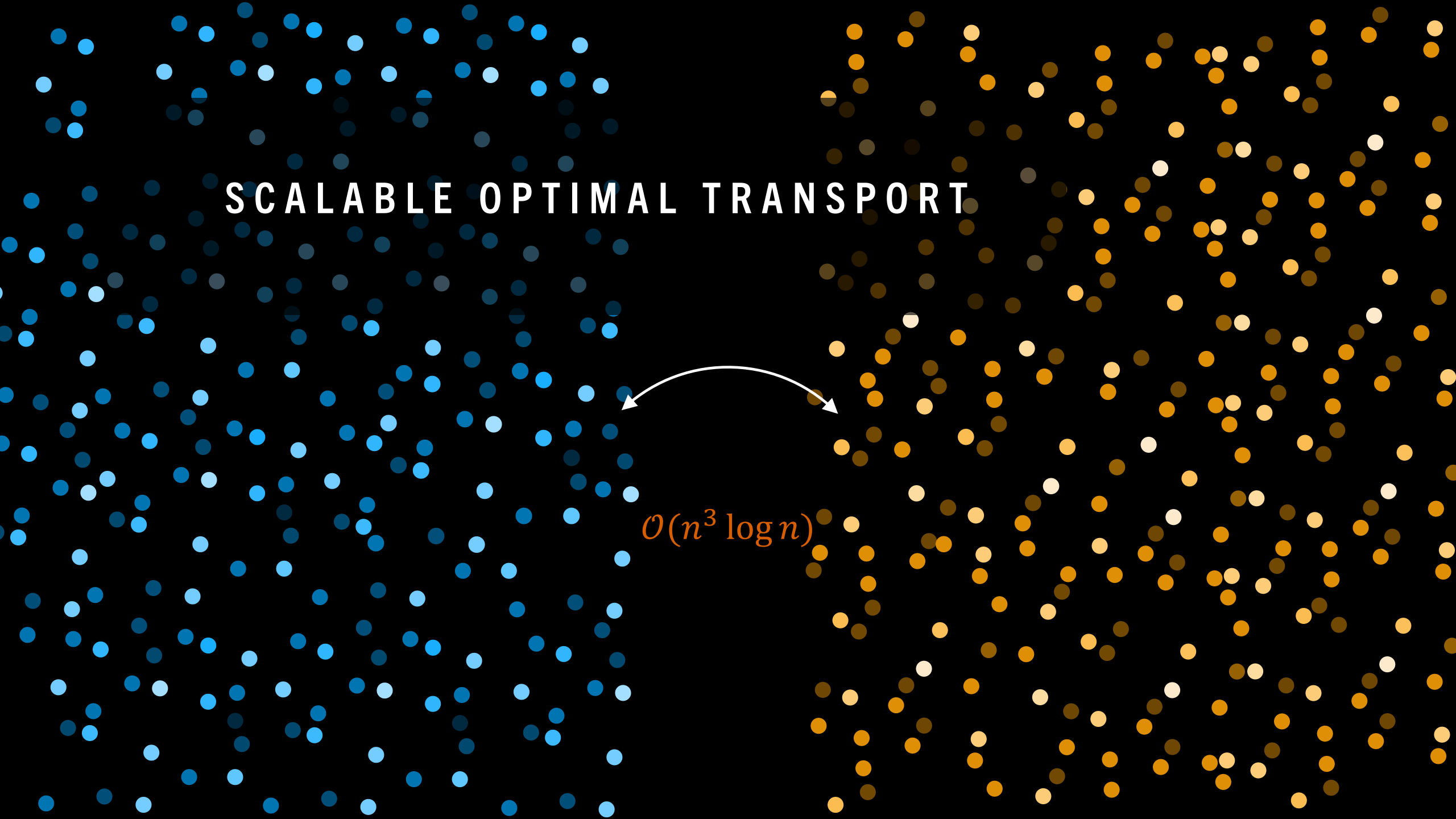
Johannes Klicpera, Marten Lienen, Stephan Günnemann

OPTIMAL TRANSPORT



DISCRETE OPTIMAL TRANSPORT




SCALABLE OPTIMAL TRANSPORT
$\mathcal{O}(n^3 \log n)$

ENTROPY-REGULARIZED OPTIMAL TRANSPORT

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

SINKHORN

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

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

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

$$\mathcal{O}(n^2)$$

SPARSE SINKHORN

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

Locality-sensitive hashing (LSH)

$$\overline{P} \approx \overline{P}^{\mathrm{sp}} = \mathrm{diag}(\overline{s})\, K^{\mathrm{sp}}\, \mathrm{diag}(\overline{t})$$

$$\mathcal{O}(n \log n)$$

LOCALLY CORRECTED NYSTRÖM SINKHORN

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

$$K_{\mathrm{Nys}} = UA^{-1}V$$

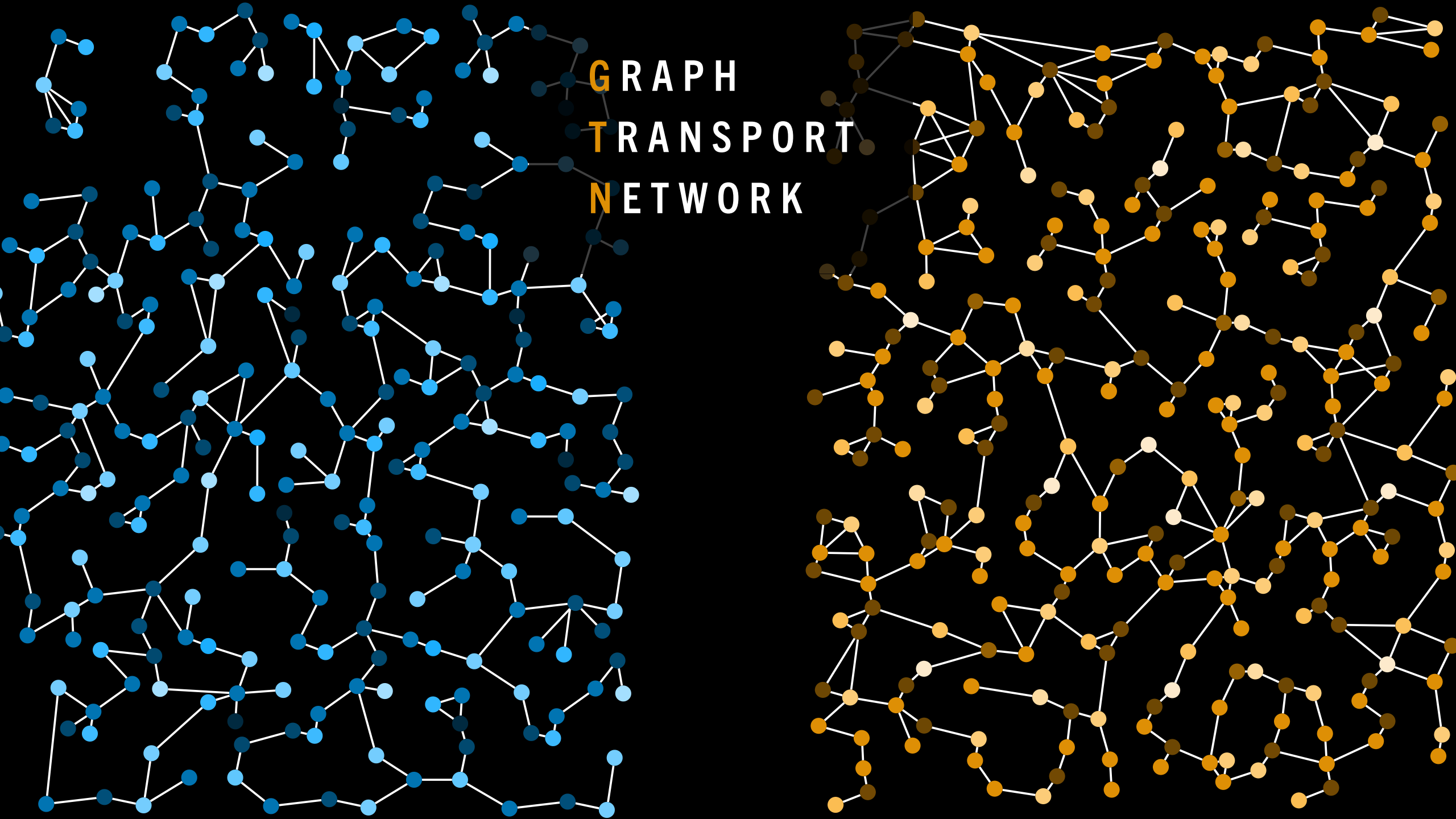
$$K_{\mathrm{LCN}} = K_{\mathrm{Nys}} - K_{\mathrm{Nys}}^{\mathrm{sp}} + K^{\mathrm{sp}}$$

general kernel approximation

Theoretically well-motivated

$O(n \log n + nl^2)$

Same convergence rate

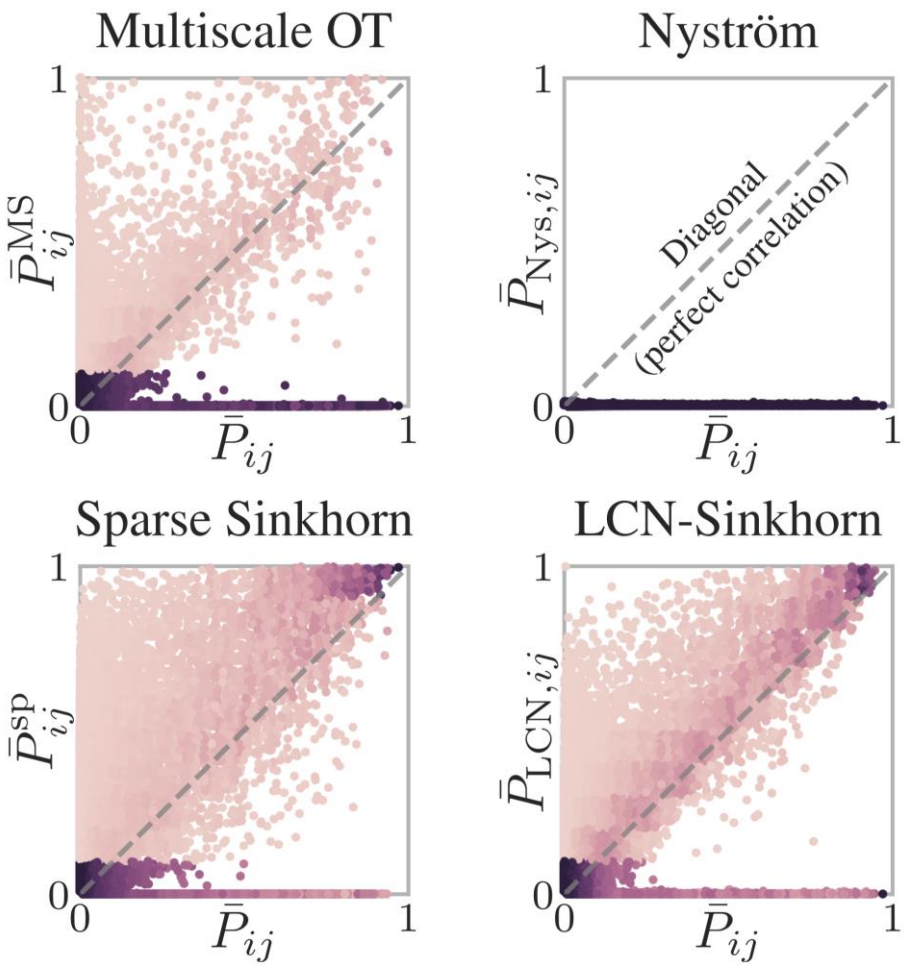

GRAPH
TRANSPORT
NETWORK

GRAPH TRANSPORT NETWORK

Graph neural network for node embeddings

Learnable unbalanced optimal transport

Multi-head optimal transport



Embedding alignment

3x faster,

+3.1pp accuracy

Graph Transport Network

- 48% error

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