

Transfer Learning on Edge Connecting Probability Estimation Under Graphon Model

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1. Introduction

- Background
- Motivation

2. Method

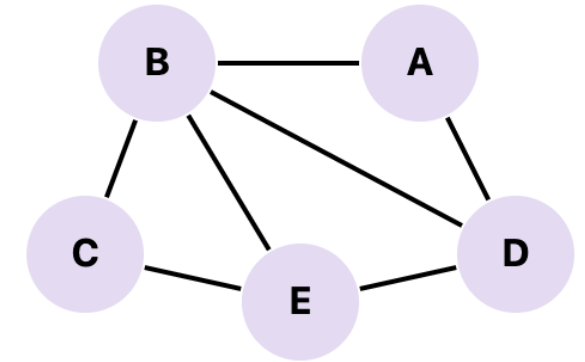
3. Experiments

4. Conclusion

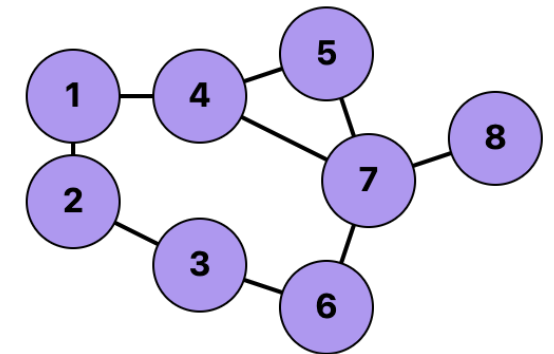
Background & Motivation

- **Edge probabilities:** Core to network modeling (social, biological, etc.); basis for link prediction, denoising, augmentation.
- **Graphon framework:** Smooth function $W: [0,1]^2 \rightarrow [0,1]$, encoding connection probabilities
- **Challenge:** Accurate graphon estimation needs large graphs; small real datasets lead to high variance.
- **Transfer idea:** Leverage related large graphs for small-graph estimation.
- **Problem:** Prior methods assume node correspondences — unrealistic.
- **Goal:** Enable correspondence-free graphon transfer with reliable alignment and negative-transfer avoidance.

Small Network



Large Network



1. Introduction

2. Method

- Overview
- Initial Graphon Estimation
- Transferring (Alignment via Optimal Transport)
- Adaptive Debiasing Mechanism

3. Experiments

4. Conclusion

Problem Setup

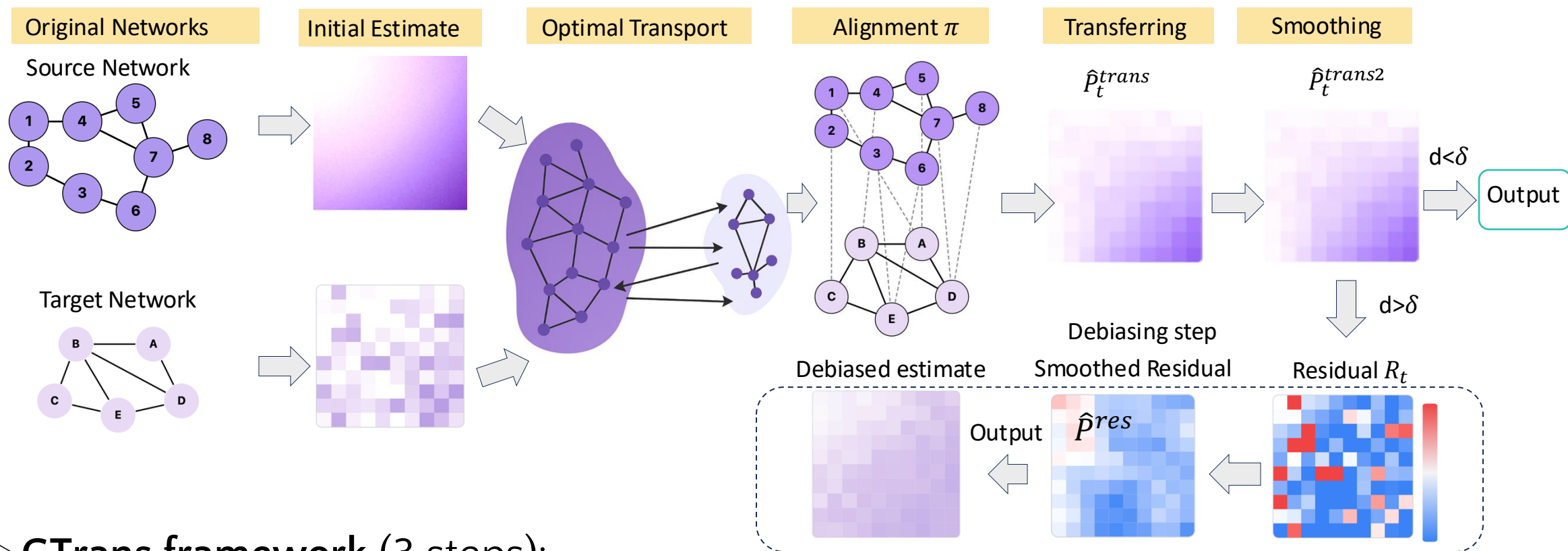
- Goal: estimate **target graphon** (latent probability matrix P_t (for small graph
- **Source graph**: adjacency $A_s \in [0,1]^{n_s \times n_s}$, $n_s > n_t$.
- **Target graph**: adjacency $A_t \in [0,1]^{n_t \times n_t}$.
- Both generated from latent graphons f_s, f_t :

$$A_{s,ij} \sim \text{Ber}\left(f_s(u_{s,i}, u_{s,j})\right), A_{t,ij} \sim \text{Ber}\left(f_t(u_{t,i}, u_{t,j})\right).$$

Objective

- Estimate P_t using **own data + transferred knowledge from source**
- Adapt to **source–target differences** to avoid negative transfer

Method-Overview: GTrans



➤ GTrans framework (3 steps):

- **Initial estimation** → Neighborhood smoothing on source & target
- **Transferring** → Align structural patterns using optimal transport,
- **Adaptive Debiasing** → Correct target-specific deviations, prevent negative transfer

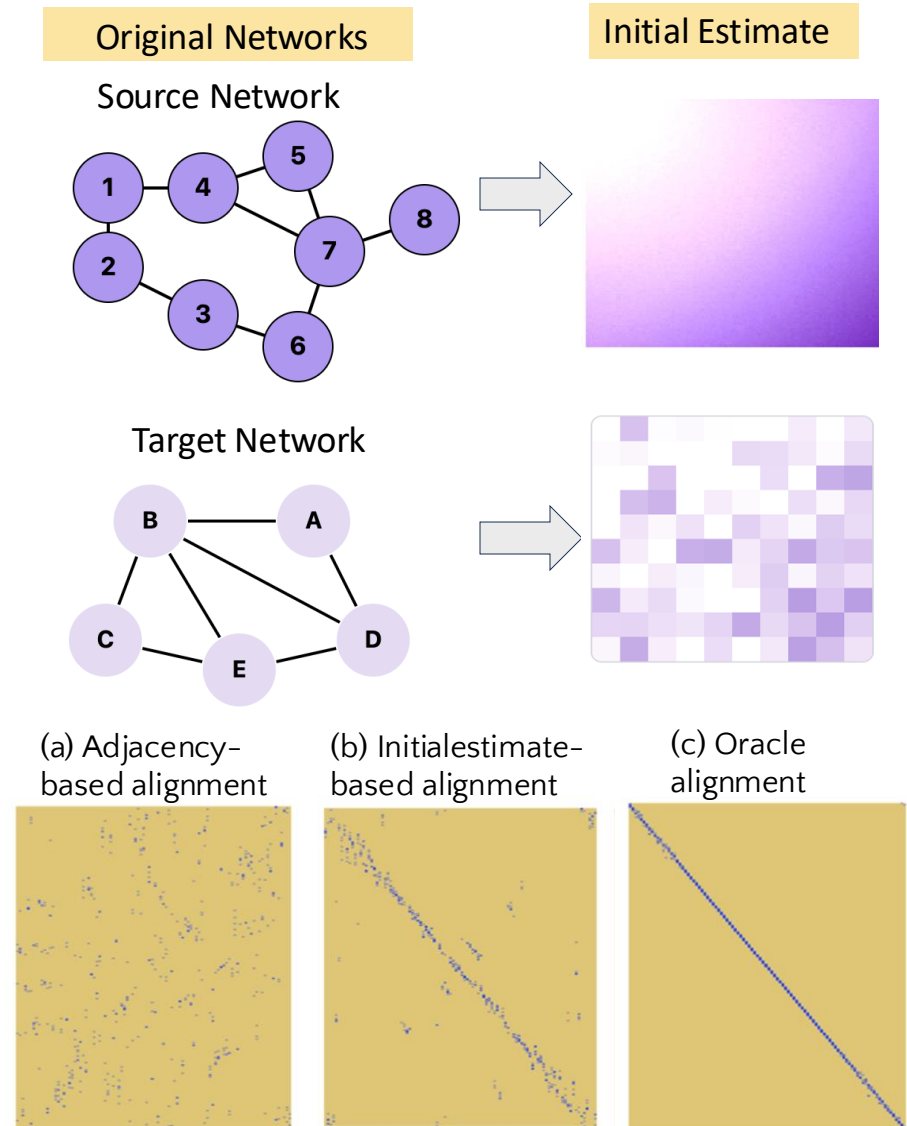
Initial Estimation Step

Initial Graphon Estimation

- **Input:** source A_s and target A_t
- **Neighborhood Smoothing (NS)** \rightarrow denoise adjacency, capture coarse:

$$\hat{P}_s^{ini} \in [0,1]^{(n_s \times n_s)}, \hat{P}_t^{ini} \in [0,1]^{(n_t \times n_t)}$$

- **Advantage:** smoother, closer to ground truth than raw adjacency
- **Limitation:** target estimate less reliable (small n_t)

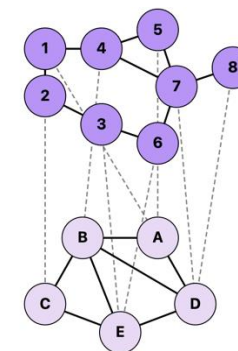


Transferring Step

Goal: Align source–target graphs and transfer structure to target space

- Optimal Transport (GW / EGW):
- Compute alignment matrix $\hat{\pi} \in [0,1]^{n_s \times n_t}$ on $\widehat{P}_s^{ini}, \widehat{P}_t^{ini}$
 - GW \rightarrow sharper alignment;
 - EGW \rightarrow more efficient for large graphs
- **Normalization:**
 - Column-normalize $\hat{\pi} \rightarrow \widetilde{\pi}$
 - $\widetilde{\pi}_{ij}$ = correspondence strength between nodes
- **Projection & Refinement**
 - Transfer: $\widehat{P}_t^{trans} = \widetilde{\pi}^T \widehat{P}_s^{ini} \widetilde{\pi}$
 - Apply smoothing $\rightarrow \widehat{P}_t^{trans2}$
 - Final estimator is **aligned + smooth**

Optimal Transport



Transferring



Smoothing



Debiasing Step

Applied If GW distance $d > \delta \rightarrow$ large domain shift, risk of negative transfer

- **Residual Computation**

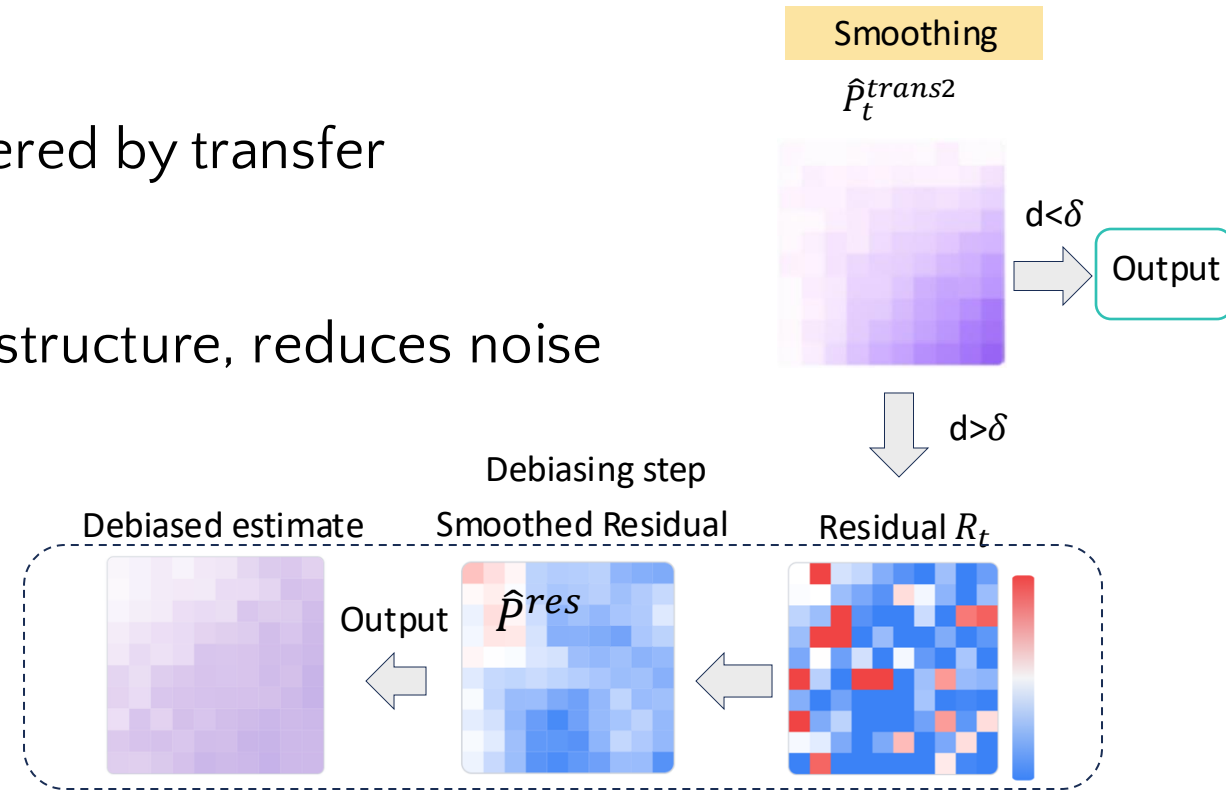
- $R_t = \widehat{P}_t^{ini} - \widehat{P}_t^{trans2}$
- captures target-specific patterns not covered by transfer

- **Residual Smoothing**

- Apply NS on $R_t \rightarrow$ denoised \widehat{P}_t^{res} ; keeps structure, reduces noise

- **Final Estimator**

- $\widehat{P}_t = \widehat{P}_t^{trans2} + \widehat{P}_t^{res}$
- If $d \leq \delta$: directly use \widehat{P}_t^{trans2}



- **Benefit:** Adaptive correction \rightarrow preserve transfer gains, avoid negative transfer

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- Link Prediction

- Graph Classification (via Data Augmentation)

4. Conclusion

Link Prediction Experiments Setup

Link prediction AUC (%): Real Networks, with source wiki-vote ($n_s = 889$):

Dataset	GTrans-GW	GTrans-EGW	NS ^[1]	USVT ^[4]	SAS ^[2]	ICE ^[3]
Dolphins ($n_t = 62$)	75.96 \pm 8.53	76.26 \pm 8.54	70.60 \pm 9.01	72.36 \pm 10.16	50.66 \pm 6.35	75.36 \pm 8.40
Firm ($n_t = 33$)	71.31 \pm 12.18	71.26 \pm 12.06	66.32 \pm 12.27	65.56 \pm 12.25	54.90 \pm 7.59	64.26 \pm 12.20
Football ($n_t = 115$)	86.64 \pm 3.66	86.74 \pm 3.72	86.75 \pm 3.49	85.32 \pm 3.56	44.56 \pm 7.38	82.46 \pm 4.59
Karate ($n_t = 34$)	82.47 \pm 10.36	82.53 \pm 10.46	76.74 \pm 12.01	71.86 \pm 15.20	63.88 \pm 11.15	80.43 \pm 11.22

➤ GTrans consistently outperforms baselines (NS, SAS, USVT, ICE)

[1] Yuan Zhang, Elizaveta Levina, and Ji Zhu. Estimating network edge probabilities by neighbourhood smoothing. *Biometrika*, 104(4):771–783, 2017.591

[2] Stanley Chan and Edoardo Airolidi. A consistent histogram estimator for exchangeable graph models. In Eric P. Xing and Tony Jebara, editors, *Proceedings of the 31st International Conference on Machine Learning*, volume 32 of *Proceedings of Machine Learning Research*, 448 pages 208–216, 22–24 Jun 2014. PMLR.449

[3]. Yichen Qin, Linhan Yu, and Yang Li. Iterative Connecting Probability Estimation for Networks. In *Advances in NeurIPS*, volume 34, pages 1155–1166, 2021

[4] Sourav Chatterjee. Matrix estimation by Universal Singular Value Thresholding. *The Annals of Statistics*, 43(1), 2015

- **Motivation:** Graph classification often suffers from **small graphs**; Graphon-based augmentation (G-Mixup) relies on accurate probability estimation → conventional estimators fail on small graphs.
- **Datasets**
 - **Targets:** IMDB-Binary, IMDB-Multi, PROTEINS-Full (all small graphs)
 - **Sources:** COLLAB (74 nodes), Reddit-Binary (429 nodes), D&D (284 nodes)
- **Baselines:**
 - **Non-Transfer baselines:** NS^[1], SAS^[2], ICE^[3], USVT^[4], GWB^[5], IGNR^[6], SIGL^[7], Graphlet Kernel^[8]
- **Evaluation Metrics:** average test accuracy over 10 runs with standard GCN classifier.

[1] Yuan Zhang, Elizaveta Levina, and Ji Zhu. Estimating network edge probabilities by neighbourhood smoothing. *Biometrika*, 104(4):771–783, 2017.591

[2] Stanley Chan and Edoardo Airolidi. A consistent histogram estimator for exchangeable graph models. In Eric P. Xing and Tony Jebara, editors, *Proceedings of the 31st International Conference on Machine Learning*, volume 32 of *Proceedings of Machine Learning Research*, 448 pages 208–216, 22–24 Jun 2014. PMLR.449

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[4] Sourav Chatterjee. Matrix estimation by Universal Singular Value Thresholding. *The Annals of Statistics*, 43(1), 2015

[5] Hongteng Xu, Dixin Luo, Lawrence Carin, and Hongyuan Zha. Learning graphons via structured gromov-wasserstein barycenters. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 35, pages 10505–10513, 2021.

[6] Xinyue Xia, Gal Mishne, and Yusu Wang. Implicit graphon neural representation. In *International Conference on Artificial Intelligence and Statistics*, pages 10619–10634. PMLR, 2023

[7] Ali Azizpour, Nicolas Zilberstein, and Santiago Segarra. Scalable implicit graphon learning. *arXiv preprint arXiv:2410.17464*, 2024.

[8] Nino Shervashidze, SVN Vishwanathan, Tobias Petri, Kurt Mehlhorn, and Karsten Borgwardt. Efficient graphlet kernels for large graph comparison. In *Artificial intelligence and statistics*, pages 488–495. PMLR, 2009

Graph Classification Results

Graph classification accuracy (%) compared against baselines

Source	Target	GTrans -GW	GTrans -EGW	NS	USVT	SAS	ICE	GWB	IGNR	SIGL	Graphlet
Reddit-B	IMDB-B	76.30	76.80	72.90	73.85	74.25	74.30	75.30	74.35	73.50	61.10
COLLAB	IMDB-B	76.25	77.50	72.90	73.85	74.25	74.30	75.30	74.35	73.50	61.10
Reddit-B	IMDB-M	49.10	51.27	43.80	48.00	44.10	43.90	47.70	47.50	49.13	39.37
COLLAB	IMDB-M	50.47	50.23	43.80	48.00	44.10	43.90	47.70	47.50	49.13	39.37
D&D	PROTEINS	69.33	68.52	63.18	65.11	65.25	65.38	63.45	65.87	67.13	70.11

GTrans-GW and **GTrans-EGW**, consistently achieves the best or comparable performance in most cases.

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➤ Understanding Gap

- Graphon estimation is unreliable on small, sparse networks.
- Existing transfer methods assume known node correspondences, which is unrealistic.
- Gap: transfer information without correspondences, while avoiding negative transfer.

➤ GTRANS Framework

- Proposed GTRANS, with three core steps
- First framework enabling robust, correspondence-free graphon transfer.

➤ **Theory:** consistency guarantees for alignment via smoothed estimators.

➤ **Experiments**

- Synthetic: outperforms baselines, robust to domain shifts.
- Real networks: Outperforms baselines in link prediction and graph classification.