GReTo: Remedying dynamic graph topology-task discordance via target homophily

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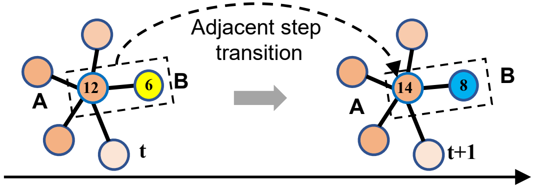
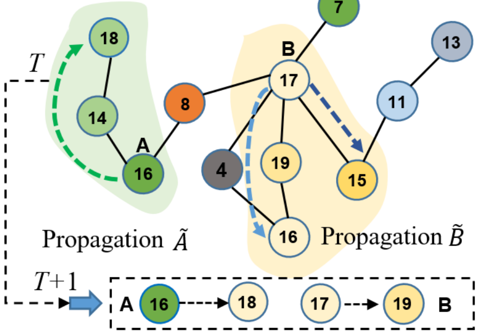
Motivation

➢ Topology-task discordance



Topology-task discordance. Neighbor B cannot facilitate aggregation from A^t to A^{t+1} but introduces noise.

Irrelevant nodes will introduce noise



Motivate target-oriented
And personalized propagation

➢ **Dynamic graph regression**: Target info can benefit effective node selection

➢ **Homophily in graphs**: Consistency between ego-node and its neighboring nodes → Neighborhood informativeness

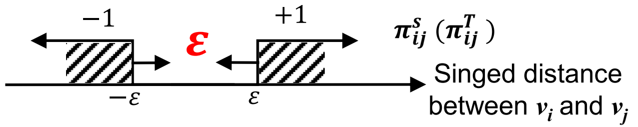
$$p_i = \frac{\sum_{v_j \in \mathcal{N}(v_i)} \mathbb{I}(y_i = y_j)}{|\mathcal{N}(v_i)|}$$

Graph homophily

Dynamic graph?

Preliminary

➢ Dynamic graph homophily



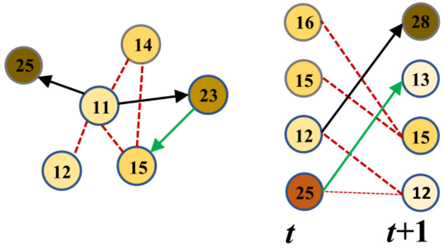
$$(\pi_{ij}^{s})_t=\begin{cases}-1, & \frac{||x_j^t||-||x_i^t||}{||x_i^t||}<-\varepsilon\\ \varepsilon, & \frac{||x_j^t-x_i^t||}{||x_i^t||}\leqslant\varepsilon\\ 1, & \frac{||x_j^t||-||x_i^t||}{||x_i^t||}>\varepsilon\end{cases}\qquad (\pi_{ij}^{T})_t=\begin{cases}-1, & \frac{||x_j^{t+1}||-||x_i^t||}{||x_i^t||}<-\varepsilon\\ \varepsilon, & \frac{||x_j^{t+1}-x_i^t||}{||x_i^t||}\leqslant\varepsilon\\ 1, & \frac{||x_j^{t+1}||-||x_i^t||}{||x_i^t||}>\varepsilon\end{cases}\quad (v_j\in\mathcal{N}(v_i))$$

Negative heterophily

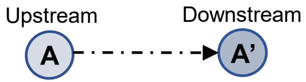
Positive heterophily

$$\pi_{v_i}(p_s,q_p,q_n)=\left[\frac{\sum_j \mathbb{I}(\pi_{ij}^{s}=\varepsilon)}{|\mathcal{N}(v_i)|},\frac{\sum_j \mathbb{I}(\pi_{ij}^{s}=1)}{|\mathcal{N}(v_i)|},\frac{\sum_j \mathbb{I}(\pi_{ij}^{s}=-1)}{|\mathcal{N}(v_i)|}\right]$$

Local neighborhood environment ➡ $\boldsymbol{LNE}_{v_i}=(d_i,p_i,q_{p_i},q_{n_i})$

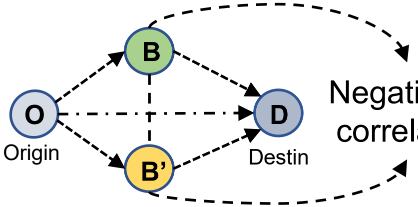


Complex spatiotemporal relations



Positively correlated

Homophily



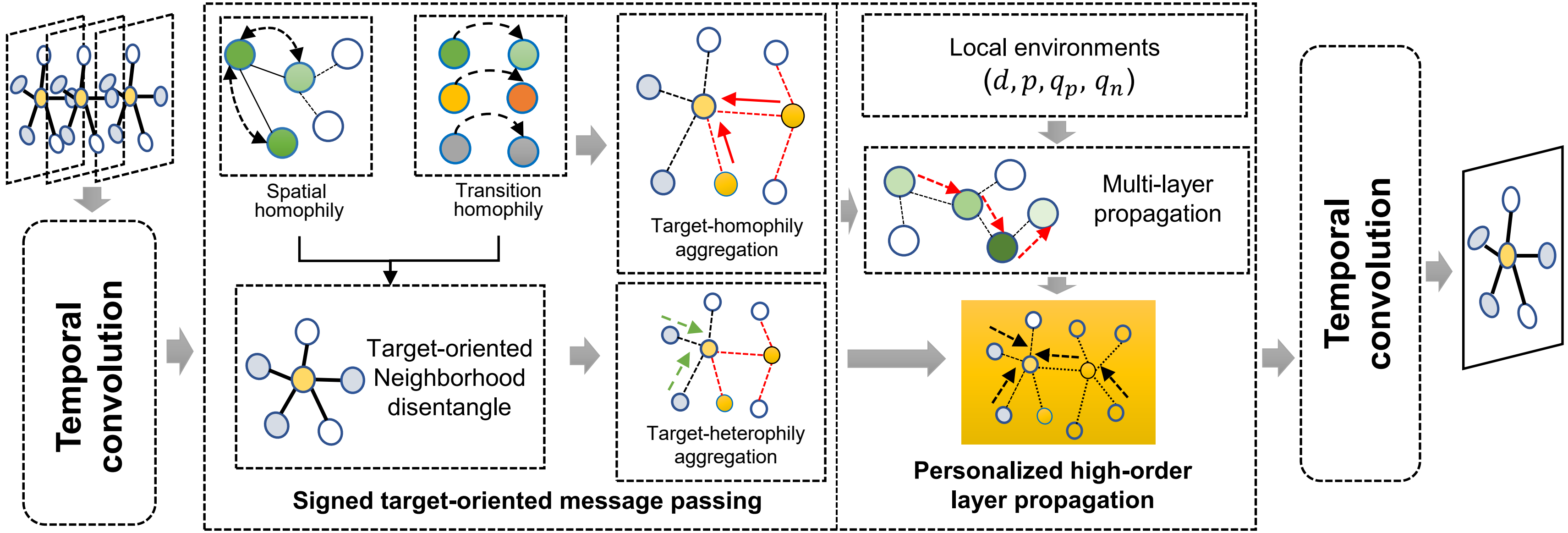
Negatively correlated

Heterophily

➡ Homophily-driven topology-task remediation

Solution

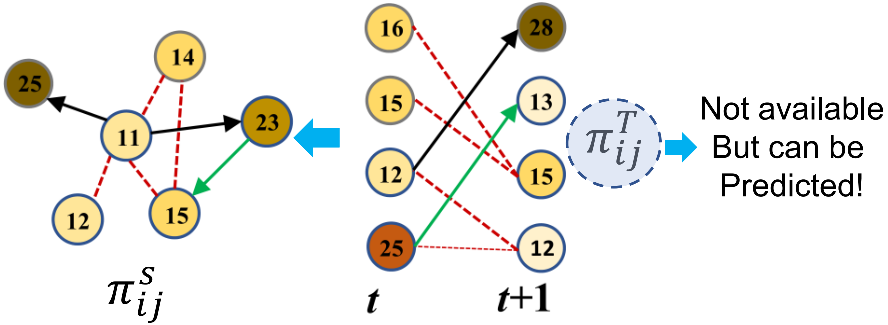
➢ **Solution: Graph learning to Remedy Topology-task discordance (GReTo)**



Solution

➢ Signed target-oriented message passing

(1) Target-homophily node selection



Intra-graph homophily

Inter-graph homophily

$$\widehat{M}_{ij} = \widehat{\pi}_{ij}^{T} \oslash \pi_{ij}^{S}$$

$$\widehat{\boldsymbol{M}} = [\widehat{\boldsymbol{M}}]_P + [\widehat{\boldsymbol{M}}]_N$$

Target-consistent nodes

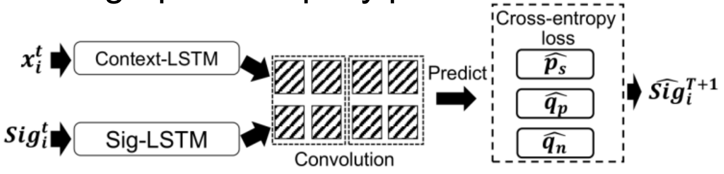
Target-deviated nodes

$$M_{ij} \in \{1, -1, -\varepsilon, \varepsilon, \frac{1}{\varepsilon}, -\frac{1}{\varepsilon}\}$$

Target-consistency contribution

Aggregation contribution

(2) Inter-graph homophily predictor



$$Sig_i^t = (\pi_{ii}^T)|_{t-1\rightarrow t}$$

$$\widehat{Sig}_R^{T+1} = \mathrm{Conv1D}(\mathrm{LSTM}(\boldsymbol{c}^1, \boldsymbol{c}^2, ..., \boldsymbol{c}^T); \mathrm{LSTM}(Sig^1, Sig^2, ..., Sig^T))$$

$$[\widehat{p},\ \widehat{q}_p,\ \widehat{q}_n]^{T+1} = \mathrm{MLP}(\widehat{Sig}_R^{T+1}; \boldsymbol{W}_s)$$

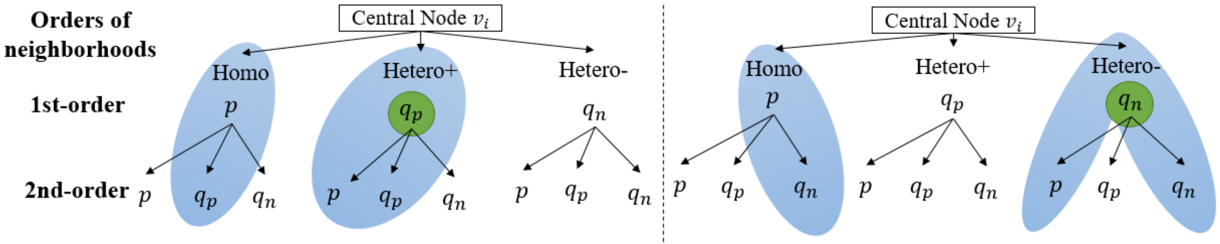
(3) Neighborhood disentangled aggregation

$$(\boldsymbol{f}_L)_i = ([\widehat{\boldsymbol{M}}]_P)_i \odot \widetilde{A}_i, \quad (\boldsymbol{f}_H)_i = ([\widehat{\boldsymbol{M}}]_N)_i \odot \widetilde{A}_i$$

$$\mathrm{AGGR}(v_i) = \alpha \sum_{j\in\mathcal{N}_L(v_i)} (\boldsymbol{f}_L)_{ij} x_j w_p + (1-\alpha) \sum_{k\in\mathcal{N}_H(v_i)} (\boldsymbol{f}_H)_{ik} x_k w_n$$

Solution

➢ Personalized high-order layer propagation



$N_+(v_i) = q_p\, d + pq_p\, d^2 + (q_p\, d \cdot (p + q_p)d)$

(a) γ is large

$N_-(v_i) = q_n\, d + pq_n\, d^2 + (q_n\, d \cdot (p + q_n)d)$

(b) γ is small

$$\begin{cases} INFO(h_i^2) > INFO(h_i^1), & 0 < q_p < \frac{1}{1+2\eta} \\ INFO(h_i^1) \geqslant INFO(h_i^2), & q_p \geqslant \frac{1}{1+2\eta} \end{cases}$$

Structure Contents

$$\phi_i^k = LiM((ND_h^k)_i, (ND_T)_i) = \frac{d_i^k \cdot MAX((ND_h^k)_i \odot (ND_T)_i)}{k}$$

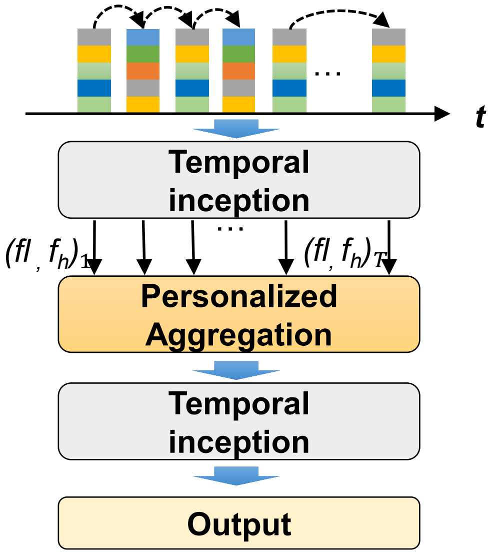
$$(ND_T)_i^t = [\hat{p},\ \hat{q}_p,\ \hat{q}_n]^t$$

$$ND_h^k = NeighH(\mathbf{A}^k \mathbf{X})$$

Selected prob decreases with layer increasing

Solution

➢ Temporal convolution learning



Sandwich spatiotemporal prediction structure

$$\widetilde{X} = \Gamma *_K X = X \odot \sigma(X); \quad H^{(K)} = f_g^*(\widetilde{X})$$

$$\widehat{Y} = \Gamma *_K H^{(K)} = H^{(K)} \odot \sigma(H^{(K)})$$

Inter-graph homophily predictor

Regression loss

$$Loss(\Theta) = -\frac{1}{N}\sum_{i=1}^{N}\Big\{\sum_{p*\in\{p,q_p,q_n\}} (p_i^* \log \widehat{p_i^*} - (1-p_i^*)\log(1-\widehat{p_i^*}))\Big\} + \frac{1}{N}\sum_{i=1}^{N}(\widehat{y}_i - y_i)^2$$

Overall loss

Experiments

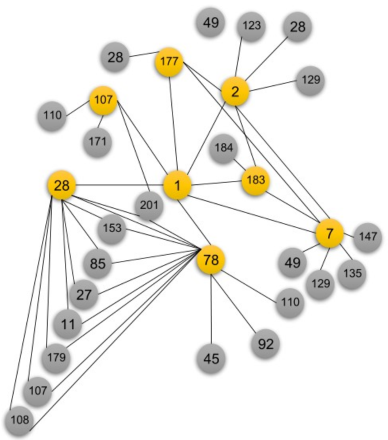
➢ Dataset statistics

	Dataset	Node #	Time step #	Time span	Interval length	Intra-graph homophily
Traffic	Metr-LA	207	34,272	03/01/2012-06/30/2012	5min	0.2273
	PeMS-Bay	325	52,116	01/01/2017-05/31/2017	5min	0.1073
Air/ Climate	KnowAir	184	11,688	01/01/2015-12/31/2018	3h	0.2481
	Temperature	184	11,688	01/01/2015-12/31/2018	3h	0.1156

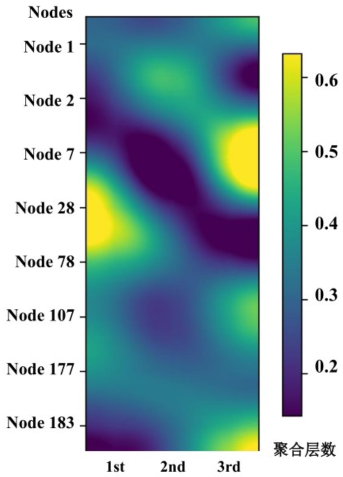
➢ Performance comparison

	Metr-LA		PeMS-Bay		KnowAir		Temperature	
	MAPE	RMSE	MAPE	RMSE	MAPE	RMSE	MAPE	RMSE
GCN	0.0975	8.3098	0.0522	4.4952	0.3146	16.5635	0.3221	1.4439
GAT	0.0628	5.8018	0.0176	1.6610	0.2435	13.3114	0.3393	1.4855
GraphSAGE	0.0606	5.7550	0.0167	1.6173	0.2449	13.1932	0.1966	1.0233
SuperGAT	0.0623	5.7886	0.0175	1.6606	0.2535	13.3671	0.3224	1.3439
EGConv	0.0609	5.7554	0.0167	1.6139	0.2399	13.2189	0.1875	1.0097
H_2GCN	0.0608	5.7292	0.0168	1.6599	0.2371	13.1207	0.1906	0.9971
STGCN	0.0554	3.8655	0.0197	1.5890	0.2437	12.3601	0.1704	1.1190
GWN	0.0528	3.8434	0.0163	1.5482	0.2288	12.8495	0.1607	0.9132
MTGNN	0.0526	3.8153	0.0170	1.5759	0.2271	12.9091	0.1682	0.9034
DCRNN	0.0532	3.8798	**0.0161**	1.5292	0.2392	13.0389	0.1351	0.9715
ASTGNN	0.0530	5.5313	0.0169	1.6229	0.2485	13.2274	0.2978	0.9330
GReTo (Ours)	**0.0500**	**3.6552**	0.0166	**1.4813**	**0.1708**	**11.0369**	**0.1341**	**0.8704**

➢ Case study



(a) Hierarchical node distribution



(b) Layer-wise importance over 3-order propagation

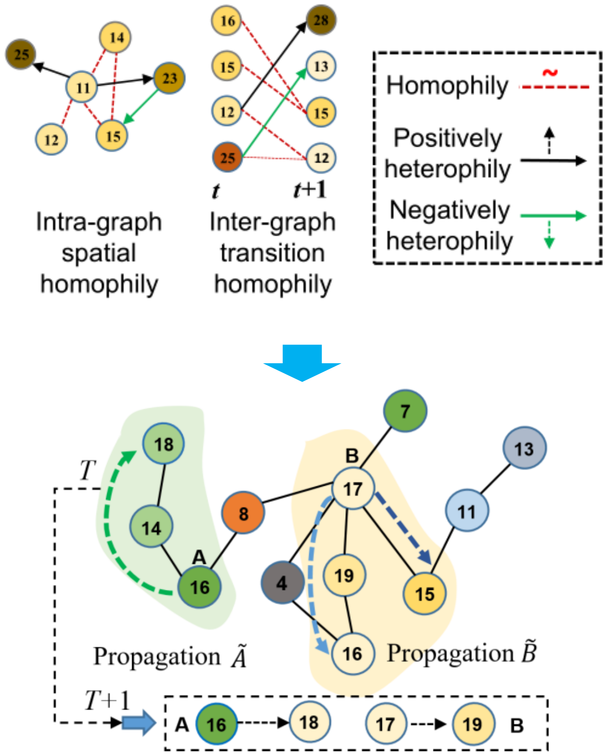
Contribution & Conclusion

➢ **Conclusion**

✓ Formalize dynamic graph homophily theory;

✓ Define target homophily via inter-graph temporal evolution

✓ Propose signed message passing and layer-wise importance measurement to realize high-order propagation over dynamic graphs



Zhou Z, et, al. Remedying Dynamic Graph Topology-task Discordance via Target Homophily, ICLR 2023.