

Balancing Consistency and Disparity in Network Alignment



Network Alignment



- Goal: To find node correspondence across networks
- An example:

Evolutionary relationship discovery				
Organism	CHIMP	MOUSE	CHICKEN	FRUIT FLY
Gene Conservation with Humans (%)	99.5	88	75	60





Problem Definition

- Given: (1) undirected networks $\mathcal{G}_1 = \{\mathcal{V}_1, A_1, X_1\}, \mathcal{G}_2 = \{\mathcal{V}_2, A_2, X_2\}$; (2) a set of anchor links \mathcal{L}
- Output: alignment matrix S







Existing Methods

- Optimization-based methods
 - Key idea: To encourage alignment consistency among neighbors
 - Example formulation (FINAL [1]):
 - Intuition: similar node pairs tend to have similar neighboring node pairs



Math:



[1] Zhang, Si, and Hanghang Tong. "Final: Fast attributed network alignment." Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining. 2016.



Existing Methods (Con't)

- Embedding-based methods
 - Key idea: To learn node embeddings w/ negative sampling
 - Example formulation [1]:
 - Intuition: Nodes that are close in embedding space are more likely to be aligned
 Encourage negative samples
 - Math:

 x_n not to be aligned with a

$$\log p(x|a) \propto \log \sigma(\mathbf{x}^T \mathbf{a}) + \sum_{m=1}^{K} E_{x_n \sim p_n(x)} \log \sigma(-\mathbf{x}_n^T \mathbf{a})$$



[1] Liu, Li, et al. "Aligning Users across Social Networks Using Network Embedding." IJCAI. 2016.

Limitation #1: Alignment Consistency



- Alignment over-smoothness issue
 - Given an anchor link (a, x), i.e., they are aligned apriori

$$\min_{\mathbf{S}} \sum_{a,b,x,y} \left[\frac{\mathbf{S}(a,x)}{\sqrt{|\mathcal{N}_{1}(a)||\mathcal{N}_{2}(x)|}} - \frac{\mathbf{S}(b,y)}{\sqrt{|\mathcal{N}_{1}(b)||\mathcal{N}_{2}(y)|}} \right]^{2} A_{1}(a,b) A_{2}(x,y)$$

- Anchor link $(a, x) \rightarrow \text{High } S(a, x)$
- Minimizing alignment difference → High S(b, y) for all neighboring node pairs
- Cannot distinguish correct alignments from misleading ones
- Equivalently, neighboring node pairs (b, y) are used as positive samples of (a, x)





Limitation #2: Alignment Disparity

- Negative sampling \rightarrow disparity \rightarrow reduce over-smoothness
- Competing sampling strategies

	Alignment consistency	Meaningful disparity	Example negative of anchor (a, x)	
Positive correlation [1]	×		Node pair (b, y)	Anchor IInk
Negative correlation [2]		×	Node pair (e, h)	\mathcal{G}_2
Degree-based sampling [3]	?	?	Node pair (d, x)	Easy negative



[1] Yang, Zhen, et al. "Understanding negative sampling in graph representation learning." KDD. 2020.
[2] Maruf, M., and Anuj Karpatne. "Maximizing Cohesion and Separation in Graph Representation Learning: A Distance-aware Negative Sampling Approach." SDM, 2021.
[3] Liu, Li, et al. "Aligning Users across Social Networks Using Network Embedding." IJCAI. 2016.



Balancing Consistency & Disparity

Key question:

What are the intrinsic relationships behind alignment consistency and disparity?

- Q1: How to design model architecture to encode alignment consistency?
- Q2: How to sample negative node pairs to distinguish correct alignments from misleading ones?
 - Target #1: Should not violate overall alignment consistency
 - Target #2: Should learn meaningful node embeddings





Outline

- Motivations
- NeXtAlign Model
 - Model Design
 - Model Training
- Experimental Results
- Conclusions





Alignment Consistency by GCNs

Unsupervised FINAL [1]



[1] Zhang, Si, and Hanghang Tong. "Final: Fast attributed network alignment." Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining. 2016.

Alignment Consistency by GCNs (Con't) $\boldsymbol{L}(a,x)=1$ Alignment consistency – semi-supervised [1] if $(a, x) \in \mathcal{L}$ $\min_{\mathbf{S}} \alpha \sum_{a,b,r,y} \left| \frac{\mathbf{S}(a,x)}{\sqrt{|\mathcal{N}_1(a)||\mathcal{N}_2(x)|}} - \frac{\mathbf{S}(b,y)}{\sqrt{|\mathcal{N}_1(b)||\mathcal{N}_2(y)|}} \right|^2 \mathbf{A}_1(a,b) \mathbf{A}_2(x,y) + (1-\alpha) \|\mathbf{S} - \mathbf{L}\|_F^2$ Fixed-point solution $S^{t} = \alpha \widetilde{A}_{1} S^{t-1} \widetilde{A}_{2} + (1-\alpha)L$ Message passing w/o parameters Alignment consistency $\boldsymbol{u}^{t} = \sqrt{\alpha} \sum_{b \in \mathcal{N}_{1}(u)} \frac{\boldsymbol{b}^{t-1}}{\sqrt{|\mathcal{N}_{1}(u)||\mathcal{N}_{1}(b)|}} + \sqrt{1-\alpha} \boldsymbol{u}^{t-1}$ $\boldsymbol{v}^{t} = \sqrt{\alpha} \sum_{y \in \mathcal{N}_{2}(v)} \frac{\boldsymbol{y}^{t-1}}{\sqrt{|\mathcal{N}_{2}(v)||\mathcal{N}_{2}(y)|}} + \sqrt{1-\alpha} \boldsymbol{v}^{t-1}$ \boldsymbol{v}^{t-1} $\boldsymbol{v}^$ $+\alpha S_1(u,a) + \sqrt{\alpha(1-\alpha)} \frac{A_1(u,a)}{\sqrt{|\mathcal{N}_1(u)||\mathcal{N}_1(a)|}}$ $a^{t} = x^{t} = \sqrt{a} \sum_{b \in \mathcal{N}_{1}(a)} \frac{b^{t-1}}{\sqrt{|\mathcal{N}_{1}(a)||\mathcal{N}_{1}(b)|}} + \sqrt{1-\alpha} x^{t-1}$ $+ \sqrt{\alpha} \sum_{y \in \mathcal{N}_{2}(x)} \frac{y^{t-1}}{\sqrt{|\mathcal{N}_{2}(x)||\mathcal{N}_{2}(y)|}} + \sqrt{1-\alpha} x^{t-1}$ $= a^{0} = x^{0} = e_{i}$ $a^{0} = x^{0} = e_{i}$ $S(a, x) = 2\alpha \widetilde{A}_{1}(a, :) L \widetilde{A}_{2}(:, x) + (1-\alpha) L(a, x) + \alpha (S_{1}(a, a) + S_{2}(x, x)) + \alpha (S_{1}(a, a) + S_{2}(x, x))$ Within-network proximity

[1] Zhang, Si, and Hanghang Tong. "Final: Fast attributed network alignment." Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining. 2016.

RelGCN – Relational GCN for Alignment

Message passing w/ parameters

$$\begin{split} \boldsymbol{u}^{t} &= \sqrt{\alpha} \sum_{b \in \mathcal{N}_{1}(u)} \frac{W_{1}^{t} \boldsymbol{b}^{t-1}}{\sqrt{|\mathcal{N}_{1}(u)||\mathcal{N}_{1}(b)|}} + \sqrt{1-\alpha} W_{0}^{t} \boldsymbol{u}^{t-1} \\ \boldsymbol{v}^{t} &= \sqrt{\alpha} \sum_{y \in \mathcal{N}_{2}(v)} \frac{W_{2}^{t} \boldsymbol{y}^{t-1}}{\sqrt{|\mathcal{N}_{2}(v)||\mathcal{N}_{2}(y)|}} + \sqrt{1-\alpha} W_{0}^{t} \boldsymbol{v}^{t-1} \\ \boldsymbol{a}^{t} &= \boldsymbol{x}^{t} = \sqrt{\alpha} \sum_{b \in \mathcal{N}_{1}(a)} \frac{W_{1}^{t} \boldsymbol{b}^{t-1}}{\sqrt{|\mathcal{N}_{1}(a)||\mathcal{N}_{1}(b)|}} + \sqrt{1-\alpha} W_{0}^{t} \boldsymbol{x}^{t-1} \\ &+ \sqrt{\alpha} \sum_{y \in \mathcal{N}_{2}(x)} \frac{W_{2}^{t} \boldsymbol{y}^{t-1}}{\sqrt{|\mathcal{N}_{2}(x)||\mathcal{N}_{2}(y)|}} \end{split}$$



- W_0^t, W_1^t, W_2^t : parameters at the *t*-th layer
- RelGCN-U: variant w/o parameters



NeXtAlign – Model Design

- Key idea:
 - Use RelGCNs to compute relative positions w.r.t. anchor nodes
 - Feed to a linear layer to compute final embeddings
- Model architecture



Model Design Details





[1] Tong, Hanghang, Christos Faloutsos, and Jia-Yu Pan. "Fast random walk with restart and its applications." Sixth international conference on data mining (ICDM'06). IEEE, 2006.
[2] Yan, Yuchen, Si Zhang, and Hanghang Tong. "BRIGHT: A Bridging Algorithm for Network Alignment." Proceedings of the Web Conference 2021, 2021.



Outline

- Motivations
- NeXtAlign Model
 - Model Design
 - Model Training
- Experimental Results
- Conclusions





NeXtAlign – Model Training

Loss functions

$$J_{a} = -\sum_{b \in \mathcal{V}_{1}} [p_{d}(b|a) \log \sigma(b'a) + kp_{n}(b|a) \log \sigma(-b'a)]$$

$$J_{x} = -\sum_{y \in \mathcal{V}_{2}} [p_{d}(y|x) \log \sigma(y'x) + kp_{n}(y|x) \log \sigma(-y'x)]$$

$$J_{ax} = -\sum_{b \in \mathcal{V}_{1}} [p_{dc}(b|x) \log \sigma(b'x) + kp_{nc}(b|x) \log \sigma(-b'x)]$$

$$-\sum_{y \in \mathcal{V}_{2}} [p_{dc}(y|a) \log \sigma(y'a) + kp_{nc}(y|a) \log \sigma(-y'a)]$$

Link prediction loss in $\mathcal{G}_1, \mathcal{G}_2$

Anchor link prediction loss

$$J = \sum_{(a,x) \in \mathcal{L}} J_{a,x} = \sum_{(a,x) \in \mathcal{L}} J_a + J_x + J_{ax}$$

- p_d , p_n : within-network positive, negative sampling distributions
- p_{dc} , p_{nc} : cross-network positive, negative sampling distributions
- Question: How to design sampling distributions?



Sampling Strategy

- An intuitive design
 - *p_d*: similar nodes are likely to co-occur in the context [1]
 - *p_n*: samples distant/dissimilar nodes [2]
 - p_{dc} : high-similarity node pairs preserve alignment consistency
 - *p_{nc}*: high-similarity node pairs → hard negative alignment pairs [3] → alignment disparity

$$\begin{split} & \text{Lemma} \quad \text{Denote } \Delta \theta_b = \theta_b^B - \theta_b^* \text{ and } \Delta \theta_y = \theta_y^B - \theta_y^*. \text{ The mean} \\ & \text{square errors for nodes } b \in \hat{\mathcal{L}}_1 \text{ and } y \in \hat{\mathcal{L}}_2 \text{ can be formulated by} \\ & \mathbb{E} \left[\Delta \theta_b^2 \right] = \frac{1}{B} \left[\frac{1}{p_d(b|a) + p_{dc}(b|x)} + \frac{1}{kp_n(b|a) + kp_{nc}(b|x)} - C \right] \\ & \mathbb{E} \left[\Delta \theta_y^2 \right] = \frac{1}{B} \left[\frac{1}{p_d(y|x) + p_{dc}(y|a)} + \frac{1}{kp_n(y|x) + kp_{nc}(y|a)} - C \right] \\ & \text{For nodes } b \in \mathcal{L}_1 \text{ and } y \in \mathcal{L}_2, \text{ the mean square error is computed by} \\ & \mathbb{E} \left[\Delta \theta_b^2 \right] = \mathbb{E} \left[\Delta \theta_y^2 \right] = \frac{1}{B} \left[\frac{1}{p_1} + \frac{1}{kp_2} - C \right] \\ \end{split}$$

Perozzi, Bryan, Rami Al-Rfou, and Steven Skiena. "Deepwalk: Online learning of social representations." KDD. 2014.
 Maruf, M., and Anuj Karpatne. "Maximizing Cohesion and Separation in Graph Representation Learning: A Distance-aware Negative Sampling Approach." SDM, 2021.
 Yang, Zhen, et al. "Understanding negative sampling in graph representation learning." KDD. 2020.



Sampling Strategy (Con't)

- Denote $\boldsymbol{b} = [\boldsymbol{b}_{(1)} || \boldsymbol{b}_{(2)}]$, $\boldsymbol{x} = [\boldsymbol{x}_{(1)} || \boldsymbol{x}_{(2)}]$
 - $b_{(1)}$: captures local information of node-b in \mathcal{G}_1
 - $b_{(2)}$: captures how node-b posits in \mathcal{G}_2
- A new scoring function \rightarrow instead of plain inner product







Outline

- Motivations
- NeXtAlign Model
 - Model Design
 - Model Training
- Experimental Results
- Conclusions





Experimental Setup

- Evaluation objectives
 - How accurate is NeXtAlign for network alignment?
 - Effectiveness of different components
- Datasets

Scenarios	Networks	# of nodes	# of edges	<pre># of attributes</pre>
S1	ACM	9,872	39,561	17
51	DBLP	9,916	44,808	17
52	Foursquare	5,313	54,233	0
52	Twitter	5,120	130,575	0
S3	Phone	1,000	41,191	0
	Email	1,003	4,627	0

- Baseline methods
 - Bright [1], NetTrans [2], FINAL [3], IONE [4], CrossMNA [5]



Yan, Yuchen, Si Zhang, and Hanghang Tong. "BRIGHT: A Bridging Algorithm for Network Alignment." WWW. 2021.
 Zhang, Si, et al. "NetTrans: Neural Cross-Network Transformation." KDD. 2020.
 Zhang, Si, and Hanghang Tong. "Final: Fast attributed network alignment." KDD. 2016.
 Liu, Li, et al. "Aligning Users across Social Networks Using Network Embedding." IJCAI. 2016.
 Chu, Xiaokai, et al. "Cross-network embedding for multi-network alignment." WWW. 2019.



Results with 20% training data w/o node attributes.

	ACM-	DBLP	Foursquare-Twitter		Phone-Email	
	Hits@10	Hits@30	Hits@10	Hits@30	Hits@10	Hits@30
NeXtAlign	$0.8417 {\pm} 0.0032$	0.9011 ± 0.0081	0.2956±0.0096	$0.4174 {\pm} 0.0066$	0.3926 ± 0.0168	$0.6748 {\pm} 0.0105$
Bright	0.7904 ± 0.0041	0.8669 ± 0.0041	0.2500 ± 0.0154	0.3206 ± 0.0097	0.2570 ± 0.0091	0.5344 ± 0.0086
NetTrans	0.7925 ± 0.0065	0.8356 ± 0.0082	0.2468 ± 0.0036	0.3458 ± 0.0098	0.2650 ± 0.0025	0.5325 ± 0.0075
FINAL	0.6768 ± 0.0080	0.8237 ± 0.0098	0.2357 ± 0.0091	0.3457 ± 0.0091	0.2203 ± 0.0151	0.4586 ± 0.0184
IONE	0.7476 ± 0.0125	0.8453 ± 0.0097	0.1624 ± 0.0109	0.2918 ± 0.0209	0.3779 ± 0.0131	0.6444 ± 0.0084
CrossMNA	0.6532 ± 0.0042	0.7900 ± 0.0041	0.0236 ± 0.0172	0.0751 ± 0.0384	0.1542 ± 0.0041	0.4045 ± 0.0115

Observations:

- Our method NeXtAlign significantly outperforms other baseline methods.
- More improvements on Foursquare-Twitter and Phone-Email whose network structures are disparate (i.e., consistency may not work well).





	10% training data		20% training data		
	Hits@10	Hits@30	Hits@10	Hits@30	
NeXtAlign	$0.785 {\pm} 0.010$	0.871±0.009	$0.872 {\pm} 0.016$	0.942 ± 0.003	
Bright	0.781 ± 0.004	0.862 ± 0.003	0.797 ± 0.004	0.870 ± 0.006	
NetTrans	0.708 ± 0.004	0.846 ± 0.009	0.841 ± 0.010	0.916 ± 0.013	
FINAL	0.651 ± 0.013	0.817 ± 0.009	0.825 ± 0.008	0.916 ± 0.006	

Results with node attributes.

Observation: Our method NeXtAlign still outperforms other baseline methods.





- Ablation study on model design
 - (1) RWR scores, (2) RelGCN-U: uses output of RelGCN-U,
 (3) RelGCN-C: uses re-scaled relative positions



Observation: All components are necessary to achieve the best performance.





Ablation study on negative sampling strategies

Hits@30 of	different	negative	sampling	strategies.

	ACM-DBLP	Foursquare-Twitter	Phone-Email
NeXtAlign	0.9277	0.4103	0.6813
Uniform	0.8975	0.3924	0.6525
Degree	0.9093	0.3923	0.6637
Positive	0.9097	0.4040	0.6650

Observation: The proposed negative sampling method achieves better performance than sampling hard negatives.





Outline

- Motivations
- NeXtAlign Model
 - Model Design
 - Model Training
- Experimental Results
- Conclusions



Conclusions

- Goal: To strike a balance of alignment consistency and disparity in semi-supervised network alignment
- Method:
 - Model design
 - Connect GCNs with FINAL
 - RelGCN for alignment consistency
 - Model training
 - New sampling method for disparity
- Results
 - NeXtAlign significantly outperforms baseline methods
 - The proposed sampling method achieves better performance



















Embedding Mean Square Errors

- Empirical risk $J^B_{(a,x)}$
 - Sample *B* nodes by p_d , p_n , p_{dc} , p_{nc}
- Denote $\boldsymbol{\theta} = [\boldsymbol{b}_1' \boldsymbol{x}, \cdots, \boldsymbol{b}_{n_1}' \boldsymbol{x}, \boldsymbol{y}_1' \boldsymbol{x}, \cdots, \boldsymbol{y}_{n_2}' \boldsymbol{x}]$
- $J_{(a,x)}^{B} = -\frac{1}{B} \sum_{i_{1},i_{2},j_{1},j_{2}} (\log \sigma(\boldsymbol{b}'_{i_{1}}\boldsymbol{x}) + \log \sigma(\boldsymbol{b}'_{i_{2}}\boldsymbol{x})$ $+ \log \sigma(\boldsymbol{y}'_{j_{1}}\boldsymbol{x}) + \log \sigma(\boldsymbol{y}'_{j_{2}}\boldsymbol{x}))$ $- \frac{1}{B} \sum_{i_{3},i_{4},j_{3},j_{4}} (\log \sigma(-\boldsymbol{b}'_{i_{3}}\boldsymbol{x}) + \log \sigma(-\boldsymbol{b}'_{i_{4}}\boldsymbol{x})$ $+ \log \sigma(-\boldsymbol{y}'_{j_{3}}\boldsymbol{x}) + \log \sigma(-\boldsymbol{y}'_{j_{4}}\boldsymbol{x}))$
- θ^*, θ^B : optimal embedding to $J_{(a,x)}, J_{(a,x)}^B$

LEMMA Denote
$$\Delta \theta_b = \theta_b^B - \theta_b^*$$
 and $\Delta \theta_y = \theta_y^B - \theta_y^*$. The mean
square errors for nodes $b \in \bar{\mathcal{L}}_1$ and $y \in \bar{\mathcal{L}}_2$ can be formulated by
 $\mathbb{E} \left[\Delta \theta_b^2 \right] = \frac{1}{B} \left[\frac{1}{p_d(b|a) + p_{dc}(b|x)} + \frac{1}{kp_n(b|a) + kp_{nc}(b|x)} - C \right]$
 $\mathbb{E} \left[\Delta \theta_y^2 \right] = \frac{1}{B} \left[\frac{1}{p_d(y|x) + p_{dc}(y|a)} + \frac{1}{kp_n(y|x) + kp_{nc}(y|a)} - C \right]$
For nodes $b \in \mathcal{L}_1$ and $y \in \mathcal{L}_2$, the mean square error is computed by
 $\mathbb{E} \left[\Delta \theta_b^2 \right] = \mathbb{E} \left[\Delta \theta_y^2 \right] = \frac{1}{B} \left[\frac{1}{p_1} + \frac{1}{kp_2} - C \right]$