Consistent Network Alignment with Node Embedding

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ABSTRACT
Network alignment, the process of finding correspondences between nodes in different graphs, has significant scientific and industrial applications. We find that many existing network alignment methods fail to achieve accurate alignments because they break up node neighborhoods during alignment, failing to preserve matched neighborhood consistency. To improve this, we propose CONE-Align, which matches nodes based on embeddings that model intra-network proximity and are aligned to be comparable across networks. Experiments on diverse, challenging datasets show that CONE-Align is robust and obtains up to 49% greater accuracy than the state-of-the-art graph alignment algorithms.

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1 INTRODUCTION
Graphs or networks are ubiquitous structures for representing complex interconnections between entities. An important problem in mining graph data is network alignment, or the task of finding correspondences between nodes in different graphs. This task has diverse, important, scientific and industrial applications, such as recommendation across social networks, pattern recognition, protein-protein interaction analysis, and database schema matching [11].

In this work, we characterize a reason why network alignment methods may fail and seek to devise solutions to it. We find that many state-of-the-art unsupervised graph alignment approaches including FINAL [20], NetAlign [1] and REGAL [10], fail to achieve matched neighborhood consistency; nodes that are close in one graph are often not matched to nodes that are close in the other graph.

To overcome this limitation, we propose CONE-Align for consistent embedding-based network alignment, utilizing well-known node embedding methods that preserve node proximities. Neighboring nodes in each graph will have similar embeddings, so when we match the embeddings, they will be mapped to similar parts of the other graph. In contrast, structural node embeddings previously used [10] do not enforce matched neighborhood consistency: neighboring nodes may not have similar structural roles, resulting in different embeddings and thus distant matchings.

The kind of node embeddings we use pose a different challenge: as there is no notion of proximity across graphs, nodes in different graphs will generally reside in different subspaces after embedding. Therefore, we require an additional step to align the graphs’ embedding subspaces before matching nodes based on embedding similarity. After doing so, however, we have the best of both worlds: matched neighborhood consistency and cross-graph comparability.

Our contributions can be summarized as follows:

- **Insights for Network Alignment:** we define the principle of matched neighborhood consistency, which motivates us to use node embedding methods with a different kind of objective than what has been used for unsupervised network alignment.
- **Principled New Method:** We propose CONE-Align for unsupervised network alignment, making node embeddings modeling intra-network proximity comparable across graphs, analogous to machine translation using monolingual word embeddings.
- **Rigorous Experiments:** We show on datasets representing diverse real-world phenomena that CONE-Align outperforms state-of-the-art methods by up to 49% in accuracy, maintaining robustness under highly challenging conditions. Key to its success is its greater ability to preserve matched neighborhood consistency.

2 RELATED WORK
We broadly characterize two relevant fields of research:

**Node Embeddings.** Node embeddings are latent feature vectors modeling relationships between nodes and/or structural characteristics, learned with various shallow and deep architectures and used for many graph mining tasks [7]. Most embedding objectives model proximity within a single graph: nearby nodes (e.g. neighbors sharing an edge or nodes with mutual neighbors) have similar features. For example, DeepWalk [16] and node2vec [9] perform random walks starting at each node to sample context nodes, using a shallow neural architecture to embed nodes similarly to their context. This process implicitly factorizes of a node pointwise mutual information matrix, which NetMF [17] instead directly factorizes.

In contrast, structural embedding methods capture a node’s structural role independent of its positional reference to specific nodes; this independence makes embeddings comparable across graphs [10]. struc2vec [18] resembles DeepWalk and node2vec but performs random walks on an auxiliary structural similarity graph.
xNetMF [10] embeddings are similar for nodes whose local neighborhoods have similar connectivity.

**Network Alignment.** Classic graph alignment approaches often formulate an optimization-based assignment problem. For example, the message-passing algorithm NetAlign [1] tries to preserve “complete squares” by matching two nodes sharing an edge in one graph to counterparts sharing an edge in the other graph. FNAL [20] optimizes a topological consistency objective which may be augmented with node and edge attribute information. Our approach is initialized by the solution to a classic convex optimization formulation [6], but to improve the accuracy, we turn to a different class of methods: those that compare node embeddings.

Nodes can be matched using embedding similarity if the embeddings in two graphs are comparable. REGAL [10] matches embeddings that capture structural roles and are comparable across graphs. BED [5] uses a principled alternative technique [8] for making embedding alignments [15] if any are known. A recent work [4] uses adversarial training techniques used in machine translation [13]. Our work uses a principled alternative technique [8] for making embedding subspaces comparable.

**3 PRELIMINARIES**

**Graphs and Embeddings.** We consider two graphs $G_1$ and $G_2$ with nodesets $\mathcal{V}_1, \mathcal{V}_2$ and adjacency matrices $A_1, A_2$ containing edges between nodes. For simplicity, we assume [10] that both graphs have $n$ nodes (if not, we can add dummy nodes to one graph). Given an embedding method, each graph $G_i$ has an $n \times d$ matrix $Y_i$ of $d$-dimensional node embeddings.

**Alignment.** An alignment between the nodes of two graphs is a function $\pi : \mathcal{V}_1 \rightarrow \mathcal{V}_2$, or alternatively a matrix $P$, where $P_{ij}$ is the (real-valued or binary) similarity between node $i$ in $G_1$ and node $j$ in $G_2$. A mapping $P$ can be found from $P$, e.g. greedy alignment $\pi(i) = \arg \max_j P_{ij}$. We assume that the graphs have a meaningful node correspondence that we seek to recover in an unsupervised setting with no node matchings known a priori.

**Neighborhood.** Let $N_{G_1}(i)$ be the neighbors of node $i$ in $G_1$, i.e., nodes that share an edge with $i$. We define node $i$’s “mapped neighborhood” in $G_2$ as the set of nodes onto which $\pi$ maps $i$’s neighbors: $N_{G_2}(i) = \{j \in \mathcal{V}_2 : \exists k \in N_{G_1}(i) \text{ s.t. } \pi(k) = j\}$. Also, we denote the neighbors of node $i$’s counterpart $\pi(i)$ as $N_{G_2}(\pi(i))$. We define the matched neighborhood consistency (MNC) of node $i$ in $G_1$ and $j$ in $G_2$ as the Jaccard similarity of the two sets:

$$MNC(i, j) = \frac{|N_{G_2}(i) \cap N_{G_2}(j)|}{|N_{G_2}(i) \cup N_{G_2}(j)|}$$

We visualize an example of MNC in Figure 1.

**4 METHOD**

We detail our proposed method CONE-Align (Fig. 2), which uses node embeddings to identify cross-graph node similarities while also preserving matched neighborhood consistency.

**4.1 Step 1: Node Embedding**

We run a node embedding method separately on each graph whose objective preserves intra-graph node proximity, i.e. neighboring nodes in each graph have similar embeddings. Thus, the embedding-based node matching will assign them to similar parts of the other graph, preserving matched neighborhood consistency.

Here, we experimentally consider NetMF [17]. It is related to DeepWalk [16] but avoids the variance introduced by random walks [10]. However, other choices are possible. We normalize the embeddings to stabilize the subsequent subspace alignment.

**4.2 Step 2: Embedding Space Alignment**

Due to the invariance of the embedding objective, the two graphs’ embeddings $Y_1 \in \mathbb{R}^{n \times d}$ and $Y_2 \in \mathbb{R}^{n \times d}$ may be translated, rotated, or rescaled relative to each other. Thus, to compare them, we must align the embedding subspaces. Inspired by unsupervised word translation [8], we jointly solve two optimization problems:

**Procrustes.** If node correspondences were known, we could find a linear embedding transformation $Q$ belonging to the set of orthogonal matrices $O^d$ by solving an orthogonal Procrustes problem:

$$\min_{Q \in O^d} ||Y_1 Q - Y_2||_2^2$$

Its solution is $Q^* = UV^\top$, where $U \Sigma V^\top$ is the SVD of $Y_1^\top Y_2$ [19].

**Wasserstein.** If the embedding space transformation were known, we could solve for the optimal node correspondence $P$ from the set of permutation matrices $P^n$ by using the Sinkhorn algorithm [3] to minimize the squared Wasserstein distance between $Y_1$ and $Y_2$:

$$\min_{P \in P^n} ||Y_1 - P Y_2||_2^2$$

**Wasserstein Procrustes.** As we know neither the transformation nor the correspondences, the problems are combined:

$$\min_{Q \in O^d} \min_{P \in P^n} ||Y_1 Q - P Y_2||_2^2$$

![Figure 2: Overview of CONE-Align. Given two graphs $G_1$ and $G_2$, we first use node embedding to model intra-graph node proximity. Second, we align the embedding spaces for cross-graph comparability. Third, we match each node in $G_1$ to the node in $G_2$ with the most similar embedding.](image-url)
We equivalently solve

where $B$ is the convex hull of $P^n$. We can find the global minimizer $P'$ with the Frank-Wolfe algorithm [5] using no iterations and Sinkhorn [3] with regularization parameter $\lambda_0$. Using $P'Y_2$, an initial $Q_0$ can be generated with orthogonal Procrustes (Eq. 2).

**Algorithm 1 Align Embeddings ($Y_1$, $Y_2$, $A_1$, $A_2$)**

1. **Input:** node embeddings $Y_1$, $Y_2$, adjacency matrices $A_1$, $A_2$, number of epochs $r$, number of iterations $s$, batch size $b$, learning rate $\eta$

2. **Convex Initialization**

3. **Stochastic Alternating Optimization**

4. **Update orthogonal transform. matrix**

5. **Return $Q, P$**

**Algorithm 2 CONE-Align ($A_1$, $A_2$, $d$, $w$, $\alpha$, $\eta$, $s$, $b$, $\gamma$)**

1. **Input:** adjacency matrices $A_1$, $A_2$

2. **For NetMF:** dimension $d$, window size $w$, # negative samples $\alpha$

3. **Other parameters as described in Alg. 1**

4. **STEP 1. Model Intra-Network Proximities with Embeddings**

5. **STEP 2. Align Embedding Spaces for Cross-Graph Comparability**

6. **STEP 3. Match Nodes with Similar Embeddings**

7. **Return $P$**

8. **Return $Q$**

9. **Return $P$**

We equivalently solve $\max_{P \in B^n} \max_{Q \in O(d)} \text{trace}(Q^T Y_1^T P Y_2) + \text{trace}(Q^T Y_2^T P Y_1) + \text{tr}(Y_1 Y_2^T P)$ with a stochastic optimization scheme [8], alternating between the Wasserstein and Procrustes problems. For $r$ epochs and $s$ iterations per epoch, we use the current embedding transformation $Q$ to find a matching $P_1$ using Sinkhorn [3] with regularization parameter $\lambda$. We then use the gradient of the Wasserstein Procrustes distance $\|Y_1 Q - P_1 Y_2 \|^2_F$ evaluated on minibatches $Y_1, Y_2$, of $b$ embeddings each, to update $Q$ using learning rate $\eta$.

**Convex Initialization.** To initialize the above nonconvex procedure, we turn to a classic convex graph matching formulation [6]:

$$\min_{P \in B^n} \| (A_1 P - PA_2) \|^2_2$$

where $B^n$ is the convex hull of $P^n$. We can find the global minimizer $P'$ with the Frank-Wolfe algorithm [5] using no iterations and Sinkhorn [3] with regularization parameter $\lambda_0$. Using $P'Y_2$, an initial $Q_0$ can be generated with orthogonal Procrustes (Eq. 2).

**Step 3: Matching Nodes with Embeddings**

After aligning the embeddings (Alg. 1) with the final transformation matrix $Q$, we match each node in $G_1$ to its nearest neighbor in $G_2$ based on Euclidean distance. As in [10], we use a $k$-d tree for fast nearest neighbor search between embedding spaces $Y_1 Q$ and $Y_2$.

We give pseudocode for CONE-Align in Alg. 2.

**5 EXPERIMENTS**

In this section, we analyze CONE-Align’s accuracy and matched neighborhood consistency in network alignment.

**5.1 Configuration of CONE-Align**

For embedding nodes, we approximate the normalized graph Laplacian with 256 eigenpairs, and set embedding dimension $d = 128$, context window size $w = 10$, and $\alpha = 1$ negative samples [17]. For the subspace alignment, we use $n_0 = 10$ iterations and regularization parameter $\lambda_0 = 1.0$ for the initial convex matching, and $r = 5$ epochs of Wasserstein Procrustes optimization with $s = 10$ iterations per epoch, batch size $b = 10$, learning rate $\eta = 1.0$, and regularization parameter $\lambda = 0.05$.

**5.2 Alignment Accuracy**

In this section, we compare the performance of CONE-Align to diverse baseline graph alignment methods on multiple datasets.

**5.2.1 Experimental Setup. Data.** We select graphs of different sizes representing various phenomena (Tab. 1). We consider the simulated-noise scenarios to create known ground truth alignments following [10]: a graph with adjacency matrix $A$ is aligned to a noisy permuted copy $A^*$. We generate a random permutation matrix $P$ and set $A^* = P A P^T$; we then randomly remove edges from $A^*$ with probability $p \in [0.05, 0.10, 0.15, 0.20, 0.25]$. Baselines. Our baselines are unsupervised methods using diverse techniques (belief propagation, spectral methods, and embeddings): (1) NetAlign [1] and (2) FINAL [20], and (3) REGAL [10].

We configure each method following the literature. NetAlign and FINAL require a matrix of prior alignment information, for which we take the top $k = \lfloor \log_2 n \rfloor$ most similar nodes by degree for each node [4, 10]. For REGAL we used recommended embedding dimension $10 \log_2 (2n)$, maximum neighbor distance 2 with discount factor $\alpha = 0.1$, and resolution parameter $\gamma_{struc} = 1$ [10].

**Metric.** We measure alignment accuracy, or the proportion of correctly aligned nodes.

**5.2.2 Results.** We report average accuracy and standard deviation over five trials for each experimental setting. In Fig. 3, we see: CONE-Align largely outperforms baselines. Note that we consider 5x noisier graphs than previous work [10]. In this challenging setting, NetAlign and FINAL achieve 10% or less accuracy. CONE-Align has higher accuracy than REGAL above 10% noise. CONE-Align is more robust to noise. We see CONE-Align’s accuracy drops more slowly as the noise increases. On the denser PPI and Facebook networks with low noise, REGAL is most accurate;
we conjecture that it is harder to model node proximities distinctly in larger neighborhoods. However, on all datasets REGAL’s accuracy drops sharply after 5% noise and falls below CONE-Align. Only CONE-Align measurably aligns the datasets at 25% noise.

5.3 Matched Neighborhood Consistency

CONE-Align models neighborhoods with proximity-preserving embedding with the goal of increasing MNC, which we now analyze.

5.3.1 Experimental Setup. Data. For brevity, we show only REGAL and CONE-Align on the Arenas dataset with 5% noise. We found that accuracy and MNC are closely related: on more challenging datasets, MNC is comparably lower.

Alignment Method Settings. We follow §5.1, §5.2.1.

Metric. We use matched neighborhood consistency (Eq. 1).

5.3.2 Results. We split the nodes into three groups by degree: $[0, \frac{N}{3}, \frac{2N}{3}, \frac{3N}{3}]$ where $N^*$ is the maximum degree. Within each group, we further distinguish correctly and incorrectly aligned nodes and visualize the distribution of MNC in Figure 4.

The box plots reveal that MNC is much higher in CONE-Align than in REGAL for nodes at all degree levels, especially for correct alignments. CONE-Align also increases MNC for misaligned nodes at low and medium degree levels, so nodes whose neighborhoods are small enough to be misaligned together may constitute a remaining failure case. However, all high-degree and most low- and medium-degree nodes are aligned accurately and consistently.

6 CONCLUSION

The success of CONE-Align offers the following takeaway to unsupervised embedding-based network alignment: the quest for cross-network embedding compatibility should not neglect intra-network proximity information. With subspace alignment, we show how to obtain the former while having the latter. Future work can explore other node embeddings, especially ones using node/edge attributes.

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