**GRAPHTSNE: A VISUALIZATION TECHNIQUE FOR GRAPH-STRUCTURED DATA**

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**ABSTRACT**

We present GraphTSNE, a novel visualization technique for graph-structured data based on t-SNE. The growing interest in graph-structured data increases the importance of gaining human insight into such datasets by means of visualization. However, among the most popular visualization techniques, classical t-SNE is not suitable on such datasets because it has no mechanism to make use of information from graph connectivity. On the other hand, standard graph visualization techniques, such as Laplacian Eigenmaps, have no mechanism to make use of information from node features. Our proposed method GraphTSNE is able to produce visualizations which account for both graph connectivity and node features. It is based on scalable and unsupervised training of a graph convolutional network on a modified t-SNE loss. By assembling a suite of evaluation metrics, we demonstrate that our method produces desirable visualizations on three benchmark datasets.

1 INTRODUCTION

Visualization of high-dimensional data has become common practice following the success of dimensionality reduction techniques such as t-SNE (van der Maaten & Hinton, 2008), Laplacian Eigenmaps (Belkin & Niyogi, 2001), and UMAP (McInnes et al., 2018). In contrast to the more general problem of dimensionality reduction, visualizations can be particularly useful as a tool to explore and hypothesize about given data. However, classical t-SNE has not been extended to handle high-dimensional data lying within an explicit graph structure, resulting in poor performance on graph-structured datasets as depicted in Figure 1. In particular, we consider datasets with two sources of information: graph connectivity between nodes and node features. Examples of graph-structured datasets include social networks, functional brain networks and gene-regulatory networks.

Formally, we consider a graph $G = (V, E)$, consisting of a set of nodes $V = \{v_i\}_{i=1}^N$, and a set of edges $E = \{(v_i, v_j)\} \subseteq V \times V$ that maps relations between nodes in $V$. In addition, each node is associated with a $n$-dimensional feature vector, given by a set of high-dimensional points $X = \{x_i \in \mathbb{R}^n\}_{i=1}^N$. The goal of visualization is to map the set of nodes $V$ to a set of low-dimensional points $\mathcal{Y} = \{y_i \in \mathbb{R}^m\}_{i=1}^N$, where $m \ll n$ and typically $m \in \{2, 3\}$.

2 RELATED WORK

**t-SNE.** t-SNE (van der Maaten & Hinton, 2008) operates by defining pairwise joint probabilities $p_{ij}$ of picking a point-pair in high-dimensional space and probabilities $q_{ij}$ of picking a point-pair in the low-dimensional map. The probabilities $p_{ij}$ of picking the pair $(x_i, x_j)$ are parametrized

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1Our implementation is available at: [https://github.com/leowyy/GraphTSNE](https://github.com/leowyy/GraphTSNE)
The objective of t-SNE is to find a low-dimensional data representation \( Y \) with mean given by the squared Euclidean distance between low-dimensional data points \( X \). Whereas the probabilities \( q_{ij} \) of picking the pair \((y_i, y_j)\) are parametrized by a normalized Student’s t-distribution given by the squared Euclidean distance between low-dimensional data points \(|y_i - y_j|^2\). The objective of t-SNE is to find a low-dimensional data representation \( \mathcal{Y} \) that minimizes the mismatch between the two probability distributions \( p_{ij} \) and \( q_{ij} \), given by the Kullback-Leibler (KL) divergence \( C_{KL} = \sum_i \sum_j p_{ij} \log \frac{p_{ij}}{q_{ij}} \).

The t-SNE loss is minimized via gradient descent on \( \frac{\partial C_{KL}}{\partial y_i} \).

**Application of t-SNE on graphs.** In the domain of graph layouts, force-directed graph drawing (Fruchterman & Reingold [1991]) considers a node placement such that the Euclidean distance between any pair of nodes in the layout is proportional to their pairwise graph-theoretic distances. Theoretical links between dimensionality reduction and graph layouts have been proposed by Yang et al. [2014]. Based on this observation, Krüger et al. [2017] have proposed a graph layout algorithm tsNET which operates similar to t-SNE, except the input distance matrix \( D \) is computed using the pairwise graph-theoretic shortest-path distances between nodes, i.e. \( D_{i,j} = \delta_G(i, j) \). However, similar to other graph layout algorithms (von Landesberger et al. [2011]), tsNET only takes the graph structure \( G \) as input and therefore, cannot leverage information provided by node features \( X \).

### 3 Method

Our method relies on two modifications to a parametric version of t-SNE proposed by van der Maaten [2009]. First, we use a graph convolutional network (GCN) (Sukhbaatar et al. [2016], Kipf & Welling [2016], Hamilton et al. [2017]) as the parametric model for the non-linear mapping between the high-dimensional data space and the low-dimensional embedding space, i.e. \( \mathcal{Y} = f_{GCN}(G, X) \). In our present work, we use a two-layer residual gated GCN of Bresson & Laurent [2018] with the following layer-wise propagation model:

\[
h_{l+1}^i = \text{ReLU} \left( U^l h_l^i + \frac{1}{|n(i)|} \sum_{j \in n(i)} \eta_{ij} \odot V^l h_j^l \right) + h_l^i, \tag{1}
\]

where \( h_l^i \) denotes the latent representation of node \( v_i \) at layer \( l \), with \( h_0^i = x_i \), \( \eta_{ij} = \sigma(A^l h_i^l + B^l h_j^l) \) denotes edge gates between the node pair \((v_i, v_j)\), with \( \sigma(\cdot) \) as the sigmoid function. \( |n(i)| \) denotes the indegree of node \( v_i \). The learnable parameters of the model are given by \( A^l, B^l, U^l, V^l \).

Second, we train our GCN using a modified t-SNE loss composed of two sub-losses: a graph clustering loss \( C_G \) and a feature clustering loss \( C_X \). Both sub-losses follow the same formulation of the classical t-SNE loss, but differ in the choice of distance metric used to compute the input pairwise distance matrix \( D \) between point-pairs. First, the graph clustering loss \( C_G \) takes as input the pairwise graph-theoretic shortest-path distances, i.e. \( D_{G}^{ij} = \delta_G(i, j) \). Second, the feature clustering loss \( C_X \) takes as input a suitable distance measure between pairs of node features, e.g. the squared Euclidean distance.
As a graph neighborhood preservation metric, we adopt the graph trustworthiness $T$ feature trustworthiness $T_S$ in the embedding neighborhoods from Martins et al. (2015), which expresses the extent to which graph neighborhoods are preserved in the low-dimensional map. We proceed with these definitions:

- **Graph neighborhood:** $S_G(v_i, r) = \{ v_j \in V \mid \delta_G(i, j) \leq r \}$; \hfill (2)  
- **Feature neighborhood:** $S_X(v_i, k) = \{ v_j \in V \mid x_j \in k \text{ nearest neighbors of } x_i \}$; \hfill (3)  
- **Embedding neighborhood:** $S_Y(v_i, k) = \{ v_j \in V \mid y_j \in k \text{ nearest neighbors of } y_i \}$ . \hfill (4)

As a graph neighborhood preservation metric, we adopt the graph trustworthiness $T_G(r)$, adapted from Martins et al. (2015), which expresses the extent to which graph neighborhoods $S_G$ are retained in the embedding neighborhoods $S_Y$. As a feature neighborhood preservation metric, we adopt the feature trustworthiness $T_X(k)$, proposed by Venna & Kaski (2006), which expresses the extent to which feature neighborhoods $S_X$ are retained in the embedding neighborhoods $S_Y$. Complete details of the trustworthiness measures are provided in Appendix B.

Next, we introduce two distance-based evaluation metrics specific to the goal of visualization. To begin, denote $K$ as the $k$-nearest neighbors graph computed by pairwise distances in the feature space for a chosen value of $k$. In our visualizations, a point-pair $(y_i, y_j)$ would ideally be placed close together in the low-dimensional map if they are either connected by an edge in the graph, i.e. $(i, j) \in E$, or have similar features, i.e. $(i, j) \in K$. Hence, a reasonable objective in visualization is to minimize the graph-based distance $P_G$ and the feature-based distance $P_X$ defined as follows:

$$P_G = \frac{1}{|E|} \sum_{(i,j) \in E} ||y_i - y_j||_2^2; \quad P_X = \frac{1}{|K|} \sum_{(i,j) \in K} ||y_i - y_j||_2^2.$$ \hfill (5, 6)

### 4.2 Results

**Quantitative assessment.** In Figure 2 we vary the weight of the graph clustering loss $\alpha \in [0, 1]$ and report the performance of the resulting visualizations. We also report the generalization accuracy of nearest-neighbor (NN) classifiers trained on the set of low-dimensional points $V$ and underlying class labels (van der Maaten, 2009). As $\alpha$ varies, GraphTSNE tradeoffs between graph and feature trustworthiness. Based only on the trustworthiness measures, it is hard to determine the optimal value of $\alpha$, which we denote as $\alpha^*$, since the measures have incomparable scales. Instead, we suggest setting $\alpha^*$ to the value of $\alpha$ with the best performance on the combined distance metric ($P_G + P_X$) or generalization accuracy (if applicable). Since we do not assume the presence of class labels during training, we use the former strategy to select $\alpha^*$.

By incorporating both graph connectivity and node features, the visualizations produced with intermediate values of $\alpha$ achieve better separation between classes and therefore, higher 1-NN generalization accuracy. This phenomenon has been well-studied in the context of semi-supervised classification (Yang et al., 2016; Kipf & Welling, 2016; Veličković et al., 2018) and unsupervised representation learning (Hamilton et al., 2017; Veličković et al., 2019).

**Qualitative assessment.** In Figure 3 we provide a visual comparison of the citation networks under three settings of $\alpha$. At $\alpha = 0$, our method reverts to pure feature clustering as in classical t-SNE.
This results in long edges that crowd the layout and poorly reflect the overall graph structure. At \( \alpha = 1 \), our method performs pure graph clustering, similar to tsNET [Kruiger et al. 2017]. This creates many tight clusters representing graph cliques, while arbitrarily placing disconnected nodes in the low-dimensional map. At the proposed value of \( \alpha^\ast \), GraphTSNE visualizations are able to accurately reflect the overall graph structure and achieve better separation between classes.

**Training time.** Similar to t-SNE, GraphTSNE runs in \( \mathcal{O}(N^2) \) time-complexity due to the computation of the input distance matrices \( D_X \) and \( D_G \). To lower the cost of this preprocessing step, we use the neighbor subsampling (NS) approach of [Hamilton et al. 2017] to train our GCNs using stochastic mini-batch gradient descent. After selecting a random mini-batch of nodes \( V_B \), NS iteratively expands the mini-batch by randomly choosing \( d(l) \) neighbors for each node at layer \( l \). For our two-layer GCNs, we set \( d = [10, 15] \), yielding a receptive field size of 150 per node. After the preprocessing step, a potential speed-up, which is not in our current implementation, would be to compute the gradients in \( \mathcal{O}(N \log N) \) time-complexity using tree-based approximation algorithms (van der Maaten 2014). In future work, we will explore GraphTSNE as an inductive visualization technique that will enable its use in larger and time-evolving graph datasets.

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Figure 3: Comparison of visualization techniques on benchmark datasets. Colors denote document class which are not provided during training. GraphTSNE visualizations are produced with $\alpha = \alpha^*$. 

Classical t-SNE (Pure Feature Clustering)

- Cora
  - Graph-based distance $P_G = 1.223$
  - Feature-based distance $P_X = 0.960$
  - Combined distance $P_G + P_X = 2.183$

- Citeseer
  - Graph-based distance $P_G = 0.870$
  - Feature-based distance $P_X = 0.856$
  - Combined distance $P_G + P_X = 1.726$

- Pubmed
  - Graph-based distance $P_G = 0.842$
  - Feature-based distance $P_X = 0.424$
  - Combined distance $P_G + P_X = 1.266$

GraphTSNE (Proposed Visualization)

- Cora
  - Graph-based distance $P_G = 0.257$
  - Feature-based distance $P_X = 1.164$
  - Combined distance $P_G + P_X = 1.421$

- Citeseer
  - Graph-based distance $P_G = 0.114$
  - Feature-based distance $P_X = 1.069$
  - Combined distance $P_G + P_X = 1.183$

- Pubmed
  - Graph-based distance $P_G = 0.159$
  - Feature-based distance $P_X = 0.743$
  - Combined distance $P_G + P_X = 0.902$

GraphTSNE visualizations are produced with $\alpha = \alpha^*$. 

tsNET (Pure Graph Clustering)

- Cora
  - Graph-based distance $P_G = 0.096$
  - Feature-based distance $P_X = 0.888$
  - Combined distance $P_G + P_X = 0.984$

- Citeseer
  - Graph-based distance $P_G = 0.048$
  - Feature-based distance $P_X = 1.721$
  - Combined distance $P_G + P_X = 1.769$

- Pubmed
  - Graph-based distance $P_G = 0.159$
  - Feature-based distance $P_X = 0.743$
  - Combined distance $P_G + P_X = 0.902$
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A Training Hyperparameters

Summary statistics for the benchmark datasets are presented in Table 1. Our method uses a residual gated GCN (Bresson & Laurent, 2018) with two graph convolutional layers. We consider different sets of hyperparameters for small datasets (|V| ≤ 10000) and larger datasets (|V| > 10000). For small datasets, we train our nets with 128 hidden units per layer for 360 epochs using full-batch gradient descent. For larger datasets, we train our nets with 256 hidden units per layer for 5 epochs using mini-batch gradient descent. At each epoch, we randomly partition the dataset into 1000 batches which are expanded with neighbor subsampling. We initialize network weights with Xavier initialization (Glorot & Bengio, 2010) and use batch normalization (Ioffe & Szegedy, 2015). We train using Adam (Kingma & Ba, 2015) with a learning rate of 0.00075. The learning rate scheduler has a decay factor of 1.25. Finally, we set the perplexity associated with the t-SNE loss to a default value of 30 for all experiments.

Table 1: Datasets statistics

| Dataset | Type    | Nodes | Edges | Classes | Features |
|---------|---------|-------|-------|---------|----------|
| CORA    | Citation| 2,708 | 5,429 | 7       | 1,433    |
| CITESEER| Citation| 3,337 | 4,732 | 6       | 3,703    |
| PUBMED  | Citation| 19,717| 44,328| 3       | 500      |

B Details of Trustworthiness Measures

Recall the following local neighborhood definitions from Section 4.1:

Graph neighborhood: \( S_G(v_i, r) = \{ v_j \in \mathcal{V} | \delta_G(i, j) \leq r \} \); 
Feature neighborhood: \( S_X(v_i, k) = \{ v_j \in \mathcal{V} | \mathbf{x}_j \in k \text{ nearest neighbors of } \mathbf{x}_i \} \);
Embedding neighborhood: \( S_Y(v_i, k) = \{ v_j \in \mathcal{V} | \mathbf{y}_j \in k \text{ nearest neighbors of } \mathbf{y}_i \} \).

The feature trustworthiness (Venna & Kaski, 2006) expresses the extent to which feature neighborhoods \( S_X \) are retained in the embedding neighborhoods \( S_Y \). The measure is defined as:

\[
T_X(k) = 1 - \frac{2}{Nk(2N - 3k - 1)} \sum_{i=1}^{N} \sum_{j \in U(v_i, k)} (r(i, j) - k),
\]

where \( r(i, j) \) denotes the rank of the low-dimensional point \( \mathbf{y}_j \) according to the pairwise distances from a given reference point \( \mathbf{y}_i \), and \( U(v_i, k) \) denotes the set of points in the embedding neighborhood of \( v_i \) but not in its feature neighborhood, i.e. \( U(v_i, k) = S_Y(v_i, k) \setminus S_X(v_i, k) \).

The graph trustworthiness, adapted from Martins et al. (2015), computes the Jaccard similarity between graph neighborhoods \( S_G \) and embedding neighborhoods \( S_Y \). Given a node \( v_i \) and a fixed value of \( r \), the graph neighborhood is defined by the \( r \)-hop neighborhood of node \( v_i \). For each node, set \( k = |S_G(v_i, r)| \). The graph neighborhood measure is defined as:

\[
T_G(r) = \frac{1}{|\mathcal{V}|} \sum_{i=1}^{N} \frac{|S_G(v_i, r) \cap S_Y(v_i, k)|}{|S_G(v_i, r) \cup S_Y(v_i, k)|}.
\]