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# Soft-Constrained Distance Preserving t-SNE

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**Abstract.** Dimension reduction is a crucial tool for high-dimensional data analysis. Many dimension reduction techniques have been proposed for preserving different properties of a given dataset. For data visualization, t-distributed stochastic neighborhood embedding (t-SNE) is a popular method due to its ability to produce nicely separated clusters. However, t-SNE suffers from some major drawbacks. In this paper, a distance preserving t-SNE (DPt-SNE) is proposed, aiming to capture the global structure of the data and simultaneously maintain its local cluster separation. The basic idea is to incorporate a set of soft constraints, i.e. relaxing expected pairwise distance preserving constraints in order to regulate the low-dimensional embedding to preserve global structure encoded in the given distance metric of input data. In addition, we introduce a scaling optimization parameter to alleviate potential issues that arise when the difference between high and low dimensional distances is too large to overcome. Experimental results on six datasets positively confirm that our DPt-SNE can better reveal global structure than t-SNE, while retaining competitive clustering separation.

**Keywords:**
t-SNE,
Distance preservation,
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## 1 Introduction

Dimension reduction (DR) is the process of embedding high-dimensional data into a low dimensional space while preserving intrinsic features of the original data. In particular, the low-dimensional data can be visualized on a scatter plot when the dimension of the embedding space is just 2 or 3. Data visualization gives out important visual insights into global and local structural properties of a dataset, such as its cluster structure and its distributional characteristics. A low-dimensional embedding is said to preserve local structure if neighboring points in the input space are still neighbors in the embedding space; the embedding is said to preserve global structure if the relative positioning or distances between neighborhoods in the input space are preserved in the embedding space [26]. Unfortunately, low-dimensional embeddings can be misleading sometimes because of unintended false clusters or incorrectly placing clusters far apart in the low-dimensional space [27]. Additionally, many DR methods are adept at preserving local structure but not global structure, or vice-versa [12]. For this reason, DR methods are typically chosen based on the intended task by the user.

Many DR methods have been proposed in the literature, each possessing unique advantages or disadvantages. One of the earliest and most successful DR methods is principal component analysis (PCA) [13], which linearly projects data onto a new coordinate

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system pointing in the directions of maximum variance [4]. While PCA is adept at linearly preserving global structure of data [1], it cannot model complex nonlinear relationships. Kernel PCA (KPCA) [20] overcomes this shortcoming by utilizing the kernel trick to handle nonlinearity in data. Manifold learning [6] is an approach to DR based on the assumption that high-dimensional data often lies on a low-dimensional manifold; thus, a low-dimensional representation of data can be obtained by projecting the data onto this manifold. Isometric feature mapping (ISOMAP) [22], one of the earliest manifold learning algorithms, estimates geodesic distances and then uses multidimensional scaling (MDS) [8] to obtain an embedding that preserves these distances. Additionally, local linear embedding (LLE) [19] models the manifold as a collection of patches, and Laplacian Eigenmaps [3] uses the spectral graph theory to obtain an embedding with locality preserving properties. Maximum variance unfolding (MVU) [28] is another local method that finds a kernel matrix by maximizing variance in the feature space while preserving angles and distances between neighbors in the original space.

These classical manifold learning methods focus on preserving raw distances, which can lead to poorly preserved neighborhood structure [26] and inadequate visualizations for complex high-dimensional data [24]. To address this issue, modern DR methods focus on preserving graph structure instead of raw distances [26]. A popular example is t-SNE [24], which models probability distributions over the high-dimensional data and the embedded data and minimizes the Kullback-Leibler (KL) divergence between the two distributions. In particular, t-SNE uses the heavy tailed Student t-distribution to model low-dimensional points, resulting in visualization with nicely separated clusters. Maximum posterior manifold embedding (MPME) [16] is a probabilistic DR framework which learns a distribution function of embedded points given a close prior distribution and preserves expected pairwise distances to additionally uncover any global skeleton structure of data. Uniform manifold approximation and projection (UMAP) [17] is a recent method which produces visualizations that rival t-SNE and additionally preserves more global structure. UMAP works by creating a graph in the high-dimensional space and then finding a graph in the low-dimensional space with the same topological structure. Moving away from local methods is TriMap [1], a modern DR method which uses a triplet constraint to capture global structure more effectively than the commonly used t-SNE and UMAP. Finally, pairwise controlled manifold approximation projection (PaCMAP) [26] is based on the desirable loss function principle and optimized via first focusing on preserving global structure and then focusing on preserving local structure.

Of those DR methods, t-SNE is commonly picked out for its impressive data visualizations. As shown in [12], t-SNE effectively preserves local structure, scoring high compared to other DR methods on metrics that measure local structure preservation like support vector machine (SVM) and k-nearest neighbor (KNN) accuracy. However, t-SNE possesses some major drawbacks, such as poor preservation of global structure, false clustering, and sensitivity to parameter selection and initialization [12]. To improve t-SNE's performance on capturing global structure, we propose incorporating soft-constrained expected pairwise distance preservation constraints to its KL cost function, similar to those of MPME. Additionally, we utilize the probabilities calculated over points in the high dimensional space as weights in the added constraints. Extensive experiments are conducted on six