Measuring Variance Propagation in t-SNE

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Abstract

T-SNE is a popular dimensionality reduction technique in Machine Learning that is used to visualize high-dimensional data. We seek to answer the question of how noise (in the form of variance) is propagated in the t-SNE embedding. Our experiments demonstrate that t-SNE does not accurately propagate variance, but that it preserves some measures of distance upto scaling.

Methods

We primarily dealt with two main cases to estimate variance propagation through the t-SNE embedding

1. Pointwise known error estimate
   - We constructed a dataset with a fixed variance for each cluster.
2. Unknown Error estimates
   - Without loss of generality, we considered the MNIST dataset. For each class, we estimated the possible values of variance using bootstrapping methods before and after the t-SNE embedding.

For both cases, we dealt with 1D vs. higher dimensional datasets similarly. Firstly, we projected the higher dimensional datasets down to 2 dimensions using PCA, which preserves variance. Second, we projected the original dataset to the same lower dimension using the t-SNE embedding. To estimate the variance for 1-D datasets, we used naïve variance estimate. When dealing with higher dimensional datasets, we used the spectral norm of the covariance matrix to compare the matrices.

Results

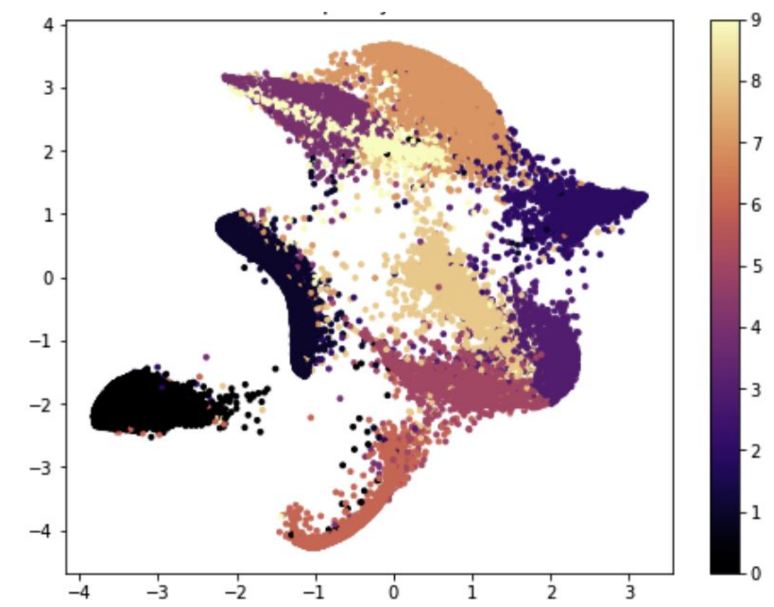

Fig 1a. A t-SNE projection of MNIST with perplexity 20

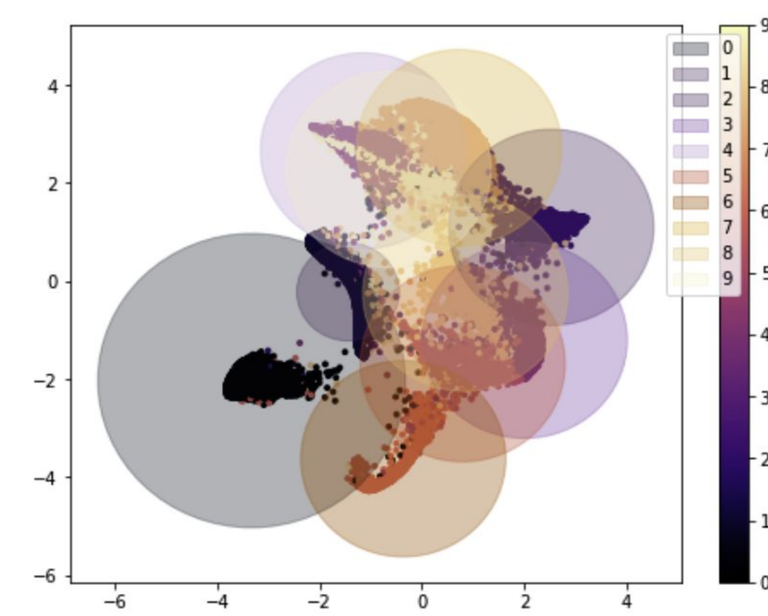

Fig 1b. Bootstrapping and Laplacian variance to envelope the uncertainty of the clustering

The Kolmogorov-Smirnov test p-value for class zero between the two histograms below was ~ 0, which indicates no correlation. The Pearson correlation metric yields the same result. This was true for other classes.

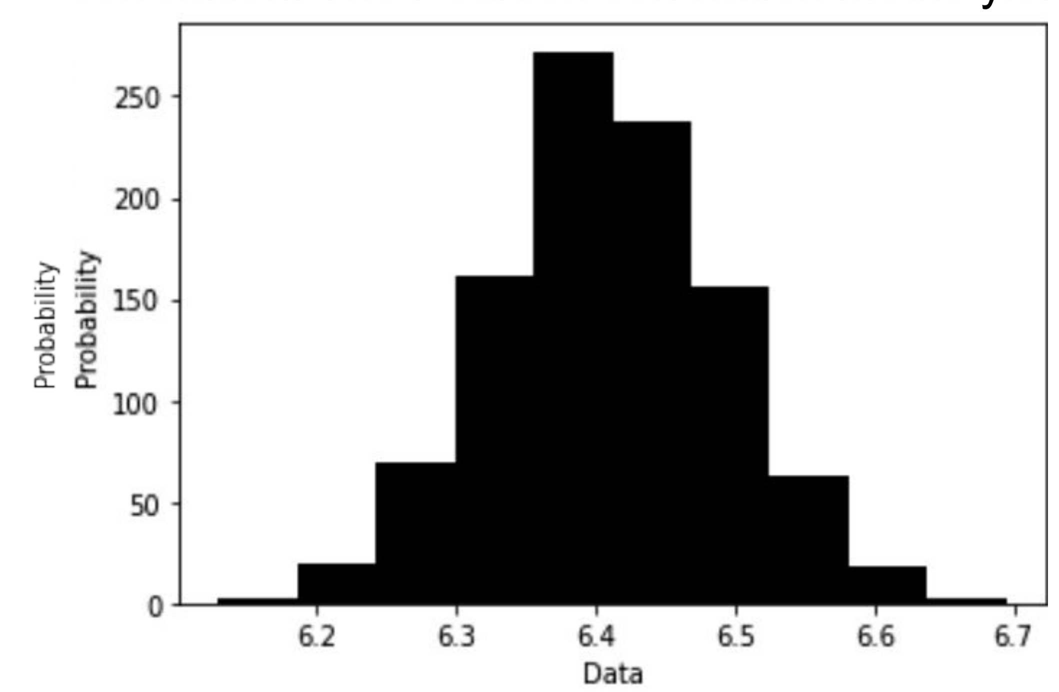

Fig 2a. Variance Histogram in 1D projection of original dataset for class 0 of MNIST

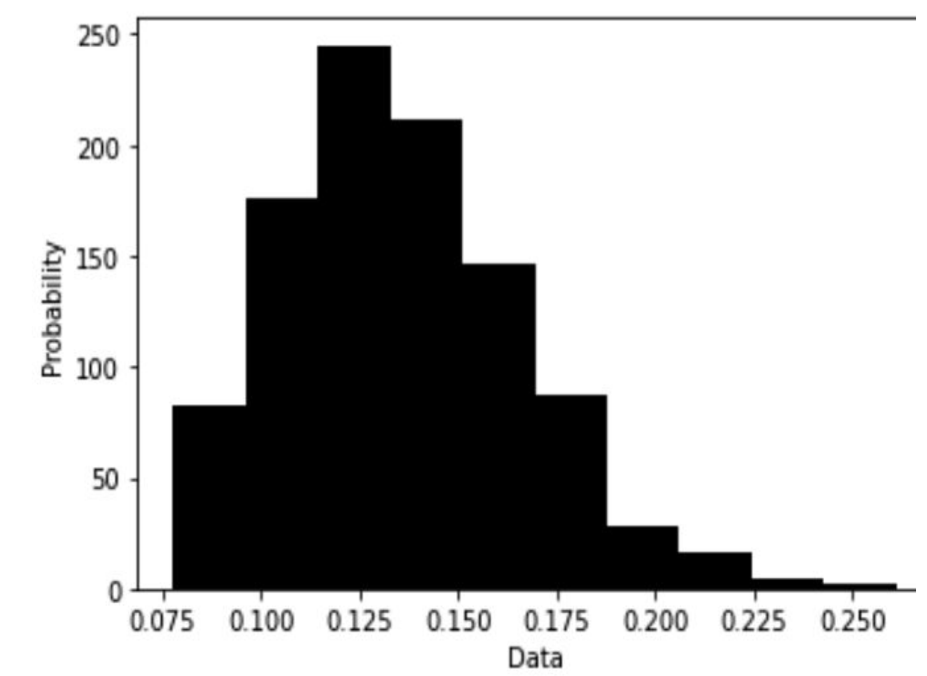

Fig 2b. Variance Histogram of 1D projected t-SNE embedding for class 0 of MNIST

We built a synthetic 20 dimensional dataset with 20 separable classes, and added random Gaussian noise to the points in each cluster. Firstly, we studied how the spectral densities of the covariance matrix of the t-SNE embeddings correlated to those of the dataset (which we obtained using PCA). Secondly, for each cluster, we studied whether the distances from the mean were correlated between the t-SNE embedding and the initial dataset.

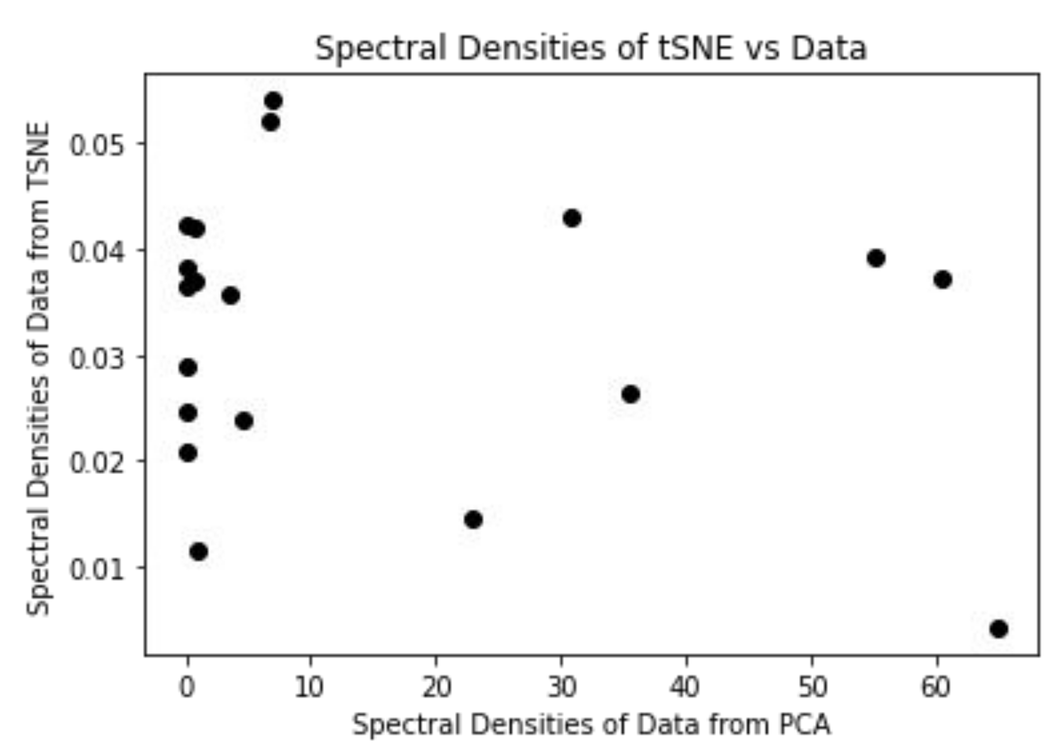

Fig 3a. The Spectral Density of the covariance matrix of the t-SNE embedding plotted against the covariance matrix of the PCA

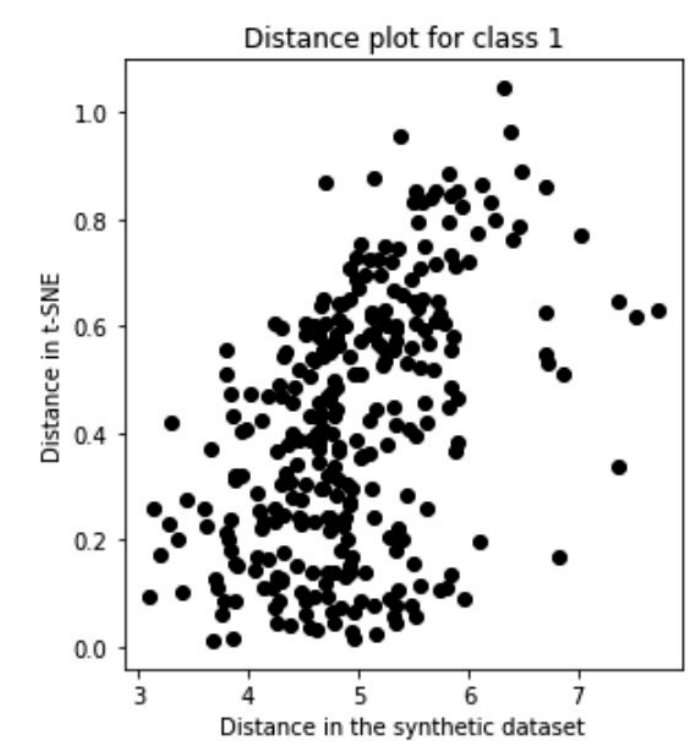

Fig 3b. The distances of each point from the mean in the t-SNE embedding versus in the initial dataset, for the cluster of class 0. There is a positive correlation.

Conclusion

1. Through this work, we effectively motivated the problem of quantifying uncertainty propagations in the t-SNE embedding.
2. We notice that in both cases of known and unknown error, t-SNE does not accurately propagate uncertainties, but that it maintains some invariant features of the dataset.
3. In the future, we hope to analytically prove that dimensionality reduction methods like t-SNE and UMAPS do not accurately propagate variance, and to do this by looking at the KL-divergence loss function.

References

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2) Geng, Y., Han, Z., Zhang, C., & Hu, Q.. (2022). Uncertainty-Aware Multi-View Representation Learning.
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