Is manifold learning reversible? Take t-SNE as an example

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Abstract

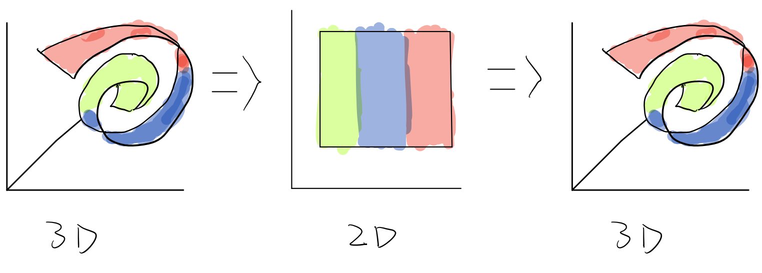
This note is about my experiment on whether manifold learning is reversible.

1 Introduction

Dimension reduction is a popular topic in statistics, and many methods have been proposed in recent years. Generally, we can divide them into two categories: linear methods and non-linear methods. Linear methods are reversible, that is, they can transform data from low-dimensional space to high-dimensional space. Hence, a question came up to my mind while doing research related to manifold learning. Can the non-linear methods be reversed?

2 My Goal

The feature of manifold learning is that it preserves the manifold structure in the process of dimensionality reduction. The classical example is the Swiss Roll from 3-dimensional space to 2-dimensional space. Thus, the very first thing we have to do is to sample a Swiss Roll dataset and try to reverse the data from 2-dimensional space (the original manifold learning result) to 3-dimensional space and see if it's still a Swiss Roll.



3 experiemnt

3.1 t-SNE as reverse method

First, we generate Swiss Roll data and color it so that we can observe:

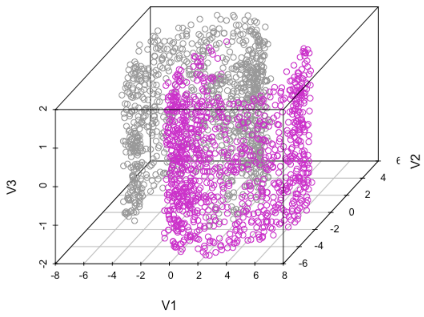


Figure 1: Swiss Roll data

Next, we do dimension reduction by t-SNE with perplexity = 55 and iteration = 200.

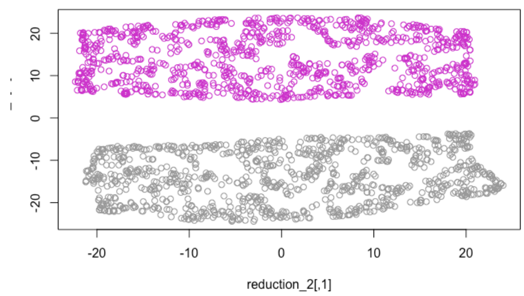


Figure 2: t-SNE result perp=55 iter = 200

By intuition, I use the t-SNE method again to transform the reduction result to 3-dimensional space with the same parameter value I use above.

We can observe that the result of the reverse still seems to retain the shape of the Swiss roll, but the thickness of the roll becomes very thin. Thus, maybe we should increase the perplexity to avoid the crowded problem.
I change perplexity to 100 and do reduction again.

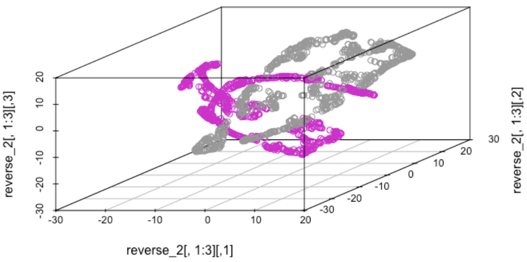


Figure 3: reverse t-SNE perp = 55 iter = 200

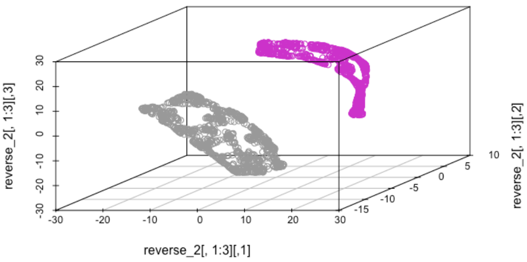


Figure 4: reverse t-SNE perp = 100 iter = 200

We can observe that the result is thicker than previous results, however, the distance between the two groups is too long to be a Swiss Roll.

3.2 SNE as reverse method

One of the reasons for the long distance of the Swiss Roll is that t-SNE changes the probability distribution in low-dimensional space from Gaussian distribution to t-distribution to solve the problem with the curse of dimensionality. Since t-distribution is heavy-tail distribution, the distance between each data point may increase. Thus, I change the t-distribution to the Gaussian distribution. That is the original SNE method.

We can see in Figure 5 that the long-distance problem between the two groups has improved. Next, we hope the shape can be more concrete.

We do the same adjustment(increase perplexity) to enhance the thickness of the reverse Swizz Roll.

We can see in Figure 6 that the SNE method has the outline of the entire roll, but the details do not have the radian of the Swiss roll. Thus, this may be the problem when we transform data from low to high-dimensional space.

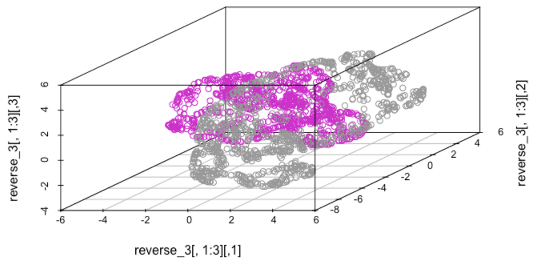


Figure 5: reverse SNE perp = 55 iter = 200 using the data in Figure 2

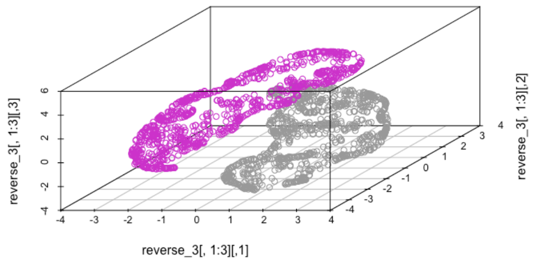


Figure 6: reverse sne perp = 150 iter = 200 using the data in Figure 2

4 Future Work

My experiment shows that the reversibility of manifold learning may work, however, the Swiss roll details can't be shown in our experiment. This is the core problem to solve in the reversibility of manifold learning that how to restore the origin details in high-dimensional space while transform data from low back to high-dimensional space.

References

[1] G. Hinton, S. Roweis, 2003, Stochastic neighbor embedding, Advances in neural information processing systems, 15, 833–840. http://citeseerx.ist.psu.edu/viewdoc/download?doi=10.1.1.13.7959&rep=rep1&type=pdf.

[2] L. van der Maaten, G. Hinton, 2008, Visualizing data using t-SNE, Journal of Machine Learning Research, 9, 2579–2605. http://www.jmlr.org/papers/v9/vandermaaten08a.html