User's Guide for t-SNE Software

Laurens van der Maaten

LVDMAATEN@GMAIL.COM

Pattern Recognition and Bioinformatics Group Delft University of Technology Mekelweg 4, 2628 CD Delft, The Netherlands

Geoffrey Hinton

HINTON@CS.TORONTO.EDU

Department of Computer Science University of Toronto 6 King's College Road, M5S 3G4 Toronto, ON, Canada

Editor:

1. Introduction

In this document, we describe the use of the t-SNE software that is publicly available online from http://lvdmaaten.github.io/lvdmaaten/tsne. Please note that this document does not describe the t-SNE technique itself; for more information on how t-SNE works, we refer to (van der Maaten and Hinton, 2008). The user's guide assumes that the Matlab environment is used, however, the discussion in section 3 is also of relevance to the use of the t-SNE software in programs that are written in, e.g., R, Java, or C++.

This document decribes two implementations of t-SNE that are available online: (1) a simple Matlab implementation, and (2) a fast binary Barnes-Hut implementation with wrappers in various languages. Implementations of t-SNE in other languages work very similarly. The use of the Matlab implementation is described in Section 2. Section 3 covers the use of the fast t-SNE implementation.

2. Simple Matlab implementation

The main purpose of the Matlab implementation of t-SNE is to illustrate how the technique works. The code contains a lot of comments, making it a useful resource in the study of the technique. Matlab's poor memory management probably makes the codes less appropriate for application on large real-world datasets. The code requires a working installation of Matlab. No additional toolboxes are required.

The syntax of the Matlab implementation of t-SNE is the following:

```
mappedX = tsne(X, labels, no_dims, init_dims, perplexity)
```

Herein, X denotes the $N \times D$ data matrix, in which rows correspond to the N instances and columns correspond to the D dimensions. In case the labels are specified, the code plots the intermediate solution every ten iterations. The labels are *only* used in the visualization of the intermediate solutions: t-SNE is an unsupervised dimensionality reduction technique. If an empty matrix ([]) is specified instead of a labels vector, no intermediate solutions are shown. The dimensionality of the visualization constructed by t-SNE can be specified through no_dims (the default value for no_dims is 2).

Before running t-SNE, the Matlab code preprocesses the data using PCA, reducing its dimensionality to init_dims dimensions (the default value is 30). The perplexity of the Gaussian distributions that are employed in the high-dimensional space can be specified through perplexity (the default value is 30). The function returns a $N \times no_dims$ matrix mappedX that specifies the coordinates of the N low-dimensional datapoints.

We illustrate the use of the simple Matlab implementation with an example. The following example requires the file mnist_train.mat as available from the t-SNE website. Notice that the example takes approximately an hour to complete.

```
% Load data
load 'mnist_train.mat'
ind = randperm(size(train_X, 1));
train_X = train_X(ind(1:5000),:);
train_labels = train_labels(ind(1:5000));
% Set parameters
no_dims = 2;
initial_dims = 50;
perplexity = 30;
% Run t-SNE
mappedX = tsne(train_X, [], no_dims, initial_dims, perplexity);
% Plot results
gscatter(mappedX(:,1), mappedX(:,2), train_labels, 'o');
```

3. Barnes-Hut Implementation

The fast Barnes-Hut implementation of t-SNE that is available online was implemented in C++. This implementation uses a different algorithm, which is described in detail by van der Maaten (2014). To compile the code, please execute the following command in the terminal:

```
cd/path/to/bhtsne
g++ sptree.cpp tsne.cpp -o bh_tsne -02
```

The code comes with a Matlab script is available that illustrates how the fast implementation of t-SNE can be used. The syntax of the Matlab script (which is called fast_tsne.m) is roughly similar to that of the tsne function. It is given by:

mappedX = fast_tsne(X, no_dims, initial_dims, perplexity, theta)

Most of the parameters are identical to those discussed in Section 2, which is why we do not discuss them in detail here. The parameter theta specified how coarse the Barnes-Hut approximation is: setting theta to 0 runs the original $\mathcal{O}(N^2)$ t-SNE algorithm, whereas using higher values runs the $\mathcal{O}(N \log N)$ with increasingly better constant. The value of theta should be between 0 and 1, and its default value is 0.5. An example of the use of the fast (landmark) version of t-SNE is given below. This example may also take up to an twenty minutes to complete.

```
% Load data
load ' mnist_train.mat'
% Set parameters
no_dims = 2;
initial_dims = 50;
perplexity = 30;
% Run t-SNE
mappedX = tsne(train_X, [], no_dims, initial_dims, perplexity);
% Plot results
gscatter(mappedX(:,1), mappedX(:,2), train_labels, ' o');
```

The example embeds all 60,000 datapoints in the MNIST training set!

There are wrappers available of the C++ code in Matlab, Python, Torch, and R. If you want to use another language, it should be fairly easy to code one up yourself. The fast implementation of t-SNE assumes the data and the parameters to be specified in a file called data.dat. The file data.dat is a binary file of which the structure is outlined in Table 1. The data matrix X should be specified as a concatenation of the instances (i.e., {instance_1, instance_2, ..., instance_N}). After executing the binary, the result of the algorithm is written in a file called result.dat, the structure of which is outlined in Table 2. The low-dimensional embedding mappedX is returned as a concatenation of instances.

Value	Number of elements	Туре
N	1	int32
D	1	int32
theta	1	double
perplexity	1	double
no_dims	1	int32
X	$N \times D$	double

Table 1: Structure of the data.dat file.

Value	Number of elements	Туре
N	1	int32
no_dims	1	int32
mappedX	$N imes \texttt{no_dims}$	double
landmarks	N	int32
costs	N	double

 Table 2: Structure of the result.dat file. The last two variables are there for legacy reasons, and need never be used.

References

- L.J.P. van der Maaten. Accelerating t-sne using tree-based algorithms. *Journal of Machine Learning Research*, 15(Oct):3221–3245, 2014.
- L.J.P. van der Maaten and G.E. Hinton. Visualizing Data using t-SNE. *Journal of Machine Learning Research*, 9(Nov):2579–2605, 2008.