t-Distributed Stochastic Embedding
Sigma Seminar, UConn
October 4, 2019

The Problem

Given a data set in a high dimensional space, about which little is known *a priori*, find structure that can be used for further study.

Example

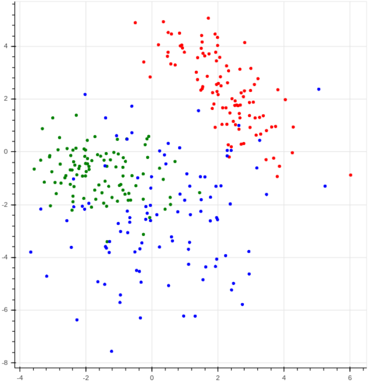
1. A single-cell RNA expression experiment produces a 10000×30000 matrix.
2. Each row of the matrix corresponds to a cell and the 30000 numbers represent the "state" of the cell.
3. One would like to identify classes of cells that are "similar" and then do further analysis to characterize what makes them so.
4. How can one extract these similar classes from the data?

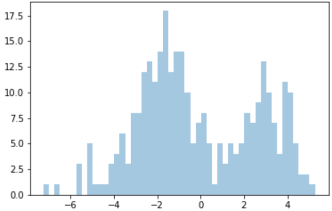
A strategy

Find a way to embed the data in 2 (or 3) dimensions while preserving as much of the structre as possible. If the two dimensional representation captures enough of the structure in the high dimensional space, then one can see patterns in the data, or use low-dimensional tools to study the data.

Principal Component Analysis

- Let X be a $k \times N$ matrix whose rows x_j correspond to samples and whose coordinates in $\mathbb{R}^N$ are particular measurements. Assume that the matrix is "centered" so that the mean of every column is zero.
- The goal of PCA is to find a linear combination of the measurements that does the best job of separating the observations.
- If w is a $N \times 1$ unit vector, then Xw gives the value of a new linear combination of measurements for each data point. The dot product $w^t X^t X w$ then measures the variance of this new measurement. So our goal is to maximize $\|w^t X^t X w\|$, and linear algebra tells us this is achieved when w is the eigenvector of $X^t X$ with maximum eigenvalue.
- More generally projecting X into the span of the top k eigenvectors captures the most significant linear variations in the data.





Original Data Projection onto Principal Direction

PCA can only detect variation in the features along linear subspaces.

More general methods

Given a $k \times N$ data matrix X, a general dimension reduction algorithm is derived from:

1. a symmetric 'similarity matrix' P whose entries p_{ij} measure the similarity of the points x_i and x_j. This could be:
    - the Euclidean distance between x_i and x_j
    - some weighted version of the Euclidean distance
    - some domain-specific measure of similarity
2. A similarity function Q that compares points y_i and y_j in $\mathbb{R}^2$ that correspond to the x_i.
3. A comparison between P and Q that measures the fidelity of the correspondence between x_i and y_i.

One tries to find points Y in $\mathbb{R}^2$ in a way that minimizes the "difference" between P and Q.

The curse of dimensionality

- The biggest obstacle to finding a good embedding of high dimensional data in a low dimensional space is that it's impossible.
- There are many ways in which high dimensional space is "different" than our intuition.

The curse of dimensionality

- The unit hypersphere in dimension n (unit ball in ℓ^2-norm) has volume $\pi^{n/2}/n\Gamma(n/2)$
- The enclosing cube (the unit ball in the ℓ^∞-norm) has volume 2^n.
- Comparing:
$$\lim_{n\to\infty} \frac{\pi^{n/2}}{n2^n\Gamma(n/2)} = 0$$
- Therefore the sphere becomes an ever smaller fraction of the cube and so bounding the coordinates of a point becomes a much weaker condition than bounding the L^2-norm.

Among many other problems, this causes "crowding" in dimensionality reduction – trying to fit too many points into small regions in $\mathbb{R}^2$.

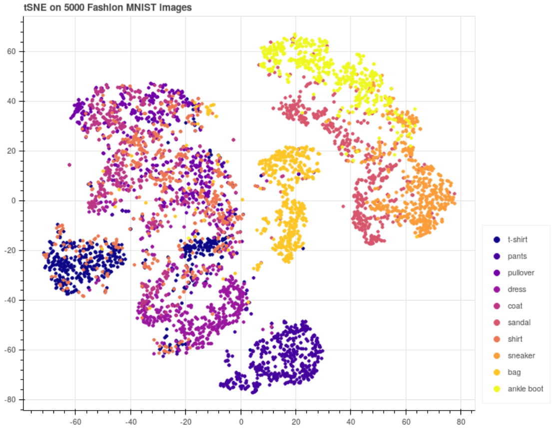
t-SNE: An example

The Fashion-MNIST data set is a collection $60k$ images of items of clothing (shirts, pants, dresses, purses, jackets, shoes). Each image is a 28×28 matrix real valued where the entries are the "darkness" of that point, from 0 being white to 1 being black.

So we may view each image as a vector in $\mathbb{R}^{784}$.

Without knowing anything about the images, what structure can we recover?

Example



tSNE on 5000 Fashion MNIST Images
60
40
20
0
-20
-40
-60
-80
-60
-40
-20
0
20
40
60
80
t-shirt
pants
pullover
dress
coat
sandal
shirt
sneaker
bag
ankle boot

Ingredients of t-SNE

Note: Before applying tSNE, one projects the data into a lower dimensional space (say, 30 or 50 dimensions) using PCA. This focuses on the most significant variation.

The main ingredients of the t-SNE algorithm are:

- A gaussian-weighted similarity function in the high dimensional space.
- A t-distributed (Cauchy-distributed) similarity function in $\mathbb{R}^2$
- The Kullback-Leibler divergence as a measure of fidelity between the two distributions
- Gradient descent as an optimization process

Gaussian similarity and perplexity

Given a point x_i in the original data set, let

$$p_{j|i}(\sigma) = \frac{e^{-\|x_j - x_i\|^2/2\sigma^2}}{Z_i(\sigma)}$$

where $Z_i(\sigma) = \sum_{k \neq i} e^{-\|x_k - x_i\|^2/2\sigma^2}$.

In some sense, $p_{j|i}(\sigma)$ measures the chance that point x_j would be selected as a neighbor for point x_i. We set $p_{i|i} = 0$.

The σ parameter controls the "reach" of the point x_i.

Perplexity

If $P = \{p_i\}$ is a discrete probability distribution, the Shannon entropy $H(P)$ of P is defined by

$$H(P) = -\sum_i p_i \log_2 p_i.$$

Entropy measures the uncertainty of the distribution; it is maximum when the p_i are all equal, and gets smaller if certain events are more likely than others. In some ideal sense, entropy is the number of bits needed to encode the output of the process.

The perplexity is defined to be $2^{H(P)}$. Since entropy measures the number of bits necessary to encode the process, perplexity is (in some sense) the effective number of states of the process.

Choosing σ_i for tSNE

The tSNE algorithm chooses the σ_i so that the perplexities of $p_{j|i}(\sigma_i)$ are all the same (and equal to some pre-set parameter).

In the original t-SNE paper, the author suggests thinking of this parameter as choosing the effective number of neighbors for each point in the dataset.
The algorithm uses a binary search for each point x_i to adjust σ_i until the perplexity is set to the preassigned value.

The high-dimensional similarity

The distance $P_{j|i}$ constructed above is not symmetric. To rectify this, the t-SNE algorithm symmetrizes it.

One way to think of this is to consider the fact that the relation "p is one of the k points closest to q" is not symmetric. Making $P_{j|i}$ symmetric is an analytic way of creating the symmetric relation "p is one of the k points closest to q, or vice versa."

This brings outlier points into fuller consideration when constructing the low-dimensional map.

The low-dimensional similarity

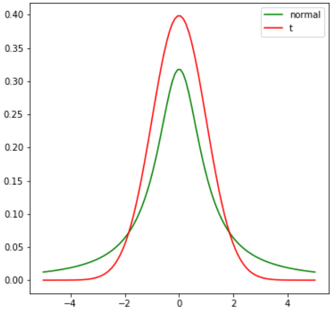
The t-SNE algorithm uses a "Cauchy Distribution" to measure similarity in the low-dimensional space. Set

$$q_{ij} = \frac{(1 + \|y_i - y_j\|^2)^{-1}}{K}$$

where $K = \sum_{k \neq l}(1 + \|y_k - y_l\|^2)^{-1}$.

This function decays much more slowly as the distance between the points grows than the gaussian does. In some sense this means the algorithm allows more "spread" in the low dimensional space than the high dimensional one to make up for the lack of "room" in the low-dimensional space.

t-distribution vs gaussian comparison



Comparing the high and low-dimensional similarity

The metric tSNE uses to compare the two similarity measures is called the Kullback-Leibler divergence or the *relative entropy.*

Given two (discrete) probability measures p and q, the KL divergence is defined as

$$KL(p||q) = -\sum_i p_i \log \frac{q_i}{p_i}$$

Note that this is not symmetric.

KL divergence

KL divergence measures the extra information required to describe data originating from the distribution p if we use the "wrong" model q to describe it.

While perhaps not particularly quantitative, one way to think of this is that the KL divergence measures how surprised we should be if the low-dimensional picture says that two points are close, but they are in fact not close in the high dimensional space.

In this sense, minimizing the KL divergence means that the low dimensional picture does the best job capturing the relationships in the high dimensional space

Unfortunately, this minimization problem may have multiple local minima.

Gradient Descent

The problem of finding local minima for the KL divergence can be attacked by gradient descent. If $f : \mathbb{R}^n \to \mathbb{R}$ is a differentiable function, then we know from multivariate calculus that the gradient

$$\nabla f = \sum_i \frac{\partial f}{\partial x_i} \mathbf{e}_i$$

points in the direction in which f increases most rapidly, and its negative points in the direction in which it decreases most rapidly.

So we can choose a small step size δ and iteratively compute

$$x^{(j+1)} = x^{(j)} - \delta \nabla f(x^{(j)})$$

until we reach a point where the gradient is small enough that $x^{(j+1)}$ and $x^{(j)}$ are almost the same.

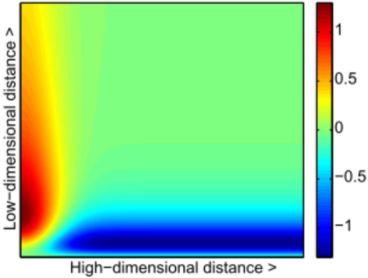
The tSNE gradient

A careful computation using the chain rule gives a formula for the gradient of the KL divergence between P and Q. Here P is fixed and we are varying the points y in the low dimensional space, and hence varying Q and then $C = KL(P||Q)$.

$$\frac{\partial C}{\partial y_i} = 4 \sum_{i,j} (p_{ij} - q_{ij})(y_i - y_j)(1 + \|y_i - y_j\|^2)^{-1}$$

The gradient (cont'd)

The gradient's dependence on the relative position of the points x_i and x_j in the high dimensional space, and y_i and y_j in the low space, is shown in this graph, taken from van der Maaten's and Hinton's original tSNE paper.



(c) Gradient of t-SNE.

There are both repulsive and attractive forces at work.

Some remarks on implementation

tSNE is an $O(N^2)$ algorithm. To make it more practical there are some modifications that yield $O(N \log N)$.

First, one can optimize the computation of the P matrix by only computing the $p_{j|i}$ for, say, the k closest points to x_i. One can efficiently find the k closest points using, for example, *vantage points trees.* These are a data structure specifically designed for this purpose.

This makes P sparse – there are only a few non-zero entries in each row.

Optimization

For the gradient descent phase, one can use a variant of the Barnes-Hut technique originally developed for computing orbital mechanics of large systems. In this approach you split the gradient into a repulsive and an attractive part:

$$\frac{\partial C}{\partial y_i} = 4(\sum_{j \neq i} p_{ij} q_{ij} Z(y_i - y_j) - \sum_{j \neq i} q_{ij}^2 Z(y_i - y_j))$$

where $q_{ij} Z = (1 + \|y_i - y_j\|^2)^{-1}$ takes constant time to compute.

The first sum requires adding terms corresponding to non-zero entries in p_{ij}, which is sparse, so this takes time $O(N)$.

Optimization

For the second term, one applies the Barnes-Hut algorithm originally used for computations in orbital mechanics of complex systems. The idea is that if a bunch of points y_i are close together, one may approximate their contribution to the force by replacing them with their center of mass.

The BH algorithm partitions space into cubes that are small enough that the center of mass of the points in each cube are a good summary of the data.

Limitations

- Gradient descent is initialized with random data, and since there are multiple local minima of the objective, different starting positions yield different results. Running the algorithm several times may give "better" or "worse" visualizations.
- There is no "map" from the higher dimensional space to the lower one; and as a result you can't compute a visualization and then add new data and see where it lies. (There is a parametric version of tSNE that addresses this problem.)
- Similarly, since there's no map, it isn't clear how to interpret the result of tSNE beyond "what you see is what you get." You can't make inferences about the original data from the low dimensional picture.

References

Hinton and van der Maaten, Visualizing High Dimensional Data with t-SNE, Journal of Machine Learning Research, 2008

van der Maaten, Accelerating t-SNE using Tree-Based Algorithms, Journal of Machine Learning Reserach, 2014.