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Rapid and brief communication

The LLE and a linear mapping

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Abstract

The locally linear embedding (LLE) is considered an effective algorithm for dimensionality reduction. In this short note, some of its key properties are studied. In particular, we show that: (1) there always exists a linear mapping from the high-dimensional space to the low-dimensional space such that all the constraint conditions in the LLE can be satisfied. The implication of the existence of such a linear mapping is that the LLE cannot guarantee a one-to-one mapping from the high-dimensional space to the low-dimensional space for a given data set; (2) if the LLE is required to globally preserve distance, it must be a PCA mapping; (3) for a given high-dimensional data set, there always exists a local distance-preserving LLE. The above results can bring some new insights into a better understanding of the LLE.

Keywords: Locally linear embedding (LLE); Linear mapping; Principal component analysis (PCA)

1. Introduction

The locally linear embedding (LLE) is considered one of effective algorithms for dimensionality reduction [1]. It has been used to solve various problems in pattern recognition [2–5]. However, to our knowledge, the LLE has the following two problems to solve:

- If two data points $\{\mathbf{z}_i, \mathbf{z}_j\}$ in the high-dimensional space are different, their corresponding data points $\{\mathbf{y}_i, \mathbf{y}_j\}$ in a lower-dimensional space must be different.
- If $\{\mathbf{z}_{i1}, \mathbf{z}_{i2}, \ldots, \mathbf{z}_{ik}\}$ are the k-neighborhood of $\mathbf{z}_i$, then $\{\mathbf{y}_{i1}, \mathbf{y}_{i2}, \ldots, \mathbf{y}_{ik}\}$ must be the k-neighborhood of $\mathbf{y}_i$.

Since the LLE does not involve any metric, in addition, taking into account our following discussions, we think the above two problems cannot completely be solved without additional constraints being further imposed.

In this note, we will show that

- There always exists a linear mapping from the $\mathbf{z}$-space to the $\mathbf{y}$-space such that all the constraint conditions in the LLE can be satisfied.
- If the LLE is required to (globally) preserve distance, it must be a principal component analysis (PCA) mapping.
- For any given high-dimensional data set, there always exists a local distance-preserving LLE.

In the note, we suppose the reader is familiar with the algorithms such as the LLE, the PCA, etc. In addition, we suppose the reader is familiar with fundamentals of matrix analysis. Besides, in this note, neither simulations nor experiments are reported, the correctness of results lie in our proofs.

2. A linear mapping from the z-space to the y-space

The following proposition shows that there always exists a linear mapping from the high-dimensional $\mathbf{z}$-space to the lower-dimensional $\mathbf{y}$-space such that all the constraint conditions in the LLE can be satisfied.

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Proposition 1. *Let* $\{\mathbf{z}_1, \mathbf{z}_2, \ldots, \mathbf{z}_m\} \subset R^n$ *be a high-dimensional data set*, $\mathbf{Z}_{n\times m} = [\mathbf{z}_1, \mathbf{z}_2, \ldots, \mathbf{z}_m]$, *if weight matrix* $\mathbf{W}_{m\times m}$ *satisfies*

$$\mathbf{1}_m^{\mathrm{T}}\mathbf{W}_{m\times m} = \mathbf{0}_m^{\mathrm{T}}, \tag{1}$$

$$\mathbf{Z}_{n\times m}\mathbf{W}_{m\times m} = \mathbf{0}_{n\times m},^{1} \tag{2}$$

then $\forall d \leqslant r(=rank(\hat{\mathbf{Z}}_{n\times m}))$, *there exists always a linear mapping* $\mathbf{A}_{d\times n}$ *and a lower-dimensional data set* $\{\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_m\} \subset R^d$ *such that* $\mathbf{Y}_{d\times m} = \mathbf{A}_{d\times n}\hat{\mathbf{Z}}_{n\times m}$, *and* $\mathbf{Y}_{d\times m}$ *satisfies all the constraint conditions in the LLE*:

$$\mathbf{Y}_{d\times m}\mathbf{W}_{m\times m} = \mathbf{0}_{d\times m}, \tag{3}$$

$$\mathbf{Y}_{d\times m}\mathbf{1}_m = \mathbf{0}_d, \tag{4}$$

$$\mathbf{Y}_{d\times m}\mathbf{Y}_{d\times m}^{\mathrm{T}} = \mathbf{I}_{d\times d}, \tag{5}$$

where

$$\mathbf{1}_m = (1, 1, \ldots, 1)^{\mathrm{T}}, \quad \mathbf{Y}_{d\times m} = [\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_m],$$

$$\hat{\mathbf{Z}}_{n\times m} = [\mathbf{z}_1 - \mathbf{z}_0, \mathbf{z}_2 - \mathbf{z}_0, \ldots, \mathbf{z}_m - \mathbf{z}_0], \quad \mathbf{z}_0 = \frac{1}{m}\sum_{j=1}^{m}\mathbf{z}_j.$$

Proof. Let $\mathbf{C}_{m\times m} = \hat{\mathbf{Z}}_{n\times m}^{\mathrm{T}}\hat{\mathbf{Z}}_{n\times m}$. Since $\hat{\mathbf{Z}}_{n\times m}\mathbf{1}_m = \mathbf{0}_n$, the 1-vector $\mathbf{1}_m$ is the eigenvector of the matrix $\mathbf{C}_{m\times m}$ for eigenvalue 0. Because $rank(\hat{\mathbf{Z}}_{n\times m}) = r$, $\hat{\mathbf{Z}}_{n\times m}$ could be decomposed by the SVD decomposition as

$$\hat{\mathbf{Z}}_{n\times m} = \mathbf{U}_{n\times r}\mathbf{\Sigma}_{r\times r}\mathbf{V}_{r\times m}, \tag{6}$$

where $\mathbf{U}_{n\times r}$ is a column-orthogonal matrix, $\mathbf{V}_{r\times m}$ a row-orthogonal matrix, and $\mathbf{\Sigma}_{r\times r}$ a diagonal matrix with positive diagonal elements. Let $\mathbf{V}_{r\times m} = [\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_m]$. Since

$$\begin{aligned}\hat{\mathbf{Z}}_{n\times m}\mathbf{W}_{m\times m} &= [\mathbf{z}_1, \mathbf{z}_2, \ldots, \mathbf{z}_m]\mathbf{W}_{m\times m} \\ &\quad - [\mathbf{z}_0, \mathbf{z}_0, \ldots, \mathbf{z}_0]\mathbf{W}_{m\times m} \\ &= \mathbf{0}_{n\times m},\end{aligned}$$

by Eq. (6) we have

$$\mathbf{V}_{r\times m}\mathbf{W}_{m\times m} = \mathbf{0}_{r\times m}. \tag{7}$$

Since $\mathbf{V}_{r\times m}$ is a row-orthogonal matrix, and in addition each of its row vectors is orthogonal to the null space of matrix $\mathbf{C}_{m\times m}$, we have

$$\mathbf{V}_{r\times m}\mathbf{V}_{r\times m}^{\mathrm{T}} = \mathbf{I}_{r\times r}, \tag{8}$$

$$\mathbf{V}_{r\times m}\mathbf{1}_m = \mathbf{0}_r. \tag{9}$$

Let $\hat{\mathbf{A}}_{r\times n} = (\mathbf{\Sigma}_{r\times r})^{-1}(\mathbf{U}_{n\times r})^{\mathrm{T}}$, then from Eq. (6), we have

$$\mathbf{V}_{r\times m} = \hat{\mathbf{A}}_{r\times n}\hat{\mathbf{Z}}_{n\times m}. \tag{10}$$

$\forall d \leqslant r$, let $\mathbf{P}_{d\times r}$ be a row-orthogonal matrix, which defines a linear mapping from r-dimensional space to d-dimensional space, for example, let $\mathbf{P}_{d\times r} = [\mathbf{I}_{d\times d}, \mathbf{0}_{d\times(r-d)}]$, then

$$\mathbf{Y}_{d\times m} = \mathbf{P}_{d\times r}\mathbf{V}_{r\times m} = (\mathbf{P}_{d\times r}\hat{\mathbf{A}}_{r\times n})\hat{\mathbf{Z}}_{n\times m}$$

and $\mathbf{Y}_{d\times m}$ satisfies the conditions (3)–(5). □

Remarks. 1. Since our mapping is a linear one, from a given data set $\{\mathbf{z}_1, \mathbf{z}_2, \ldots, \mathbf{z}_m\} \subset R^n$, we can always obtain its corresponding set $\{\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_m\} \subset R^d$ $(d < r)$, but a one-to-one correspondence cannot be guaranteed between the two sets. In other words, by the linear mapping, we can only guarantee that in the r-dimensional space, if two data points $\{\mathbf{z}_i, \mathbf{z}_j\}$ are different, their corresponding $\{\mathbf{y}_i, \mathbf{y}_j\} \subset R^r$ must be different, not in the $d(< r)$-dimensional space.

2. Since the constraint conditions on set $\{\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_m\}$ obtained by this proposition are identical to those in the LLE, our linear mapping must be included in the LLE. By this reasoning, we think the two problems outlined at the beginning of this comment cannot be solved without further conditions being imposed.

3. The relationship between our linear mapping and the LLE

In Remark 2 of the above section, we indicate that our linear mapping must be included in the LLE. In this section, some specifics of the relationship between the linear mapping and the LLE will be provided.

Proposition 2. *Let* $N_l(\mathbf{W}_{m\times m})$ *be the left null space of* $\mathbf{W}_{m\times m}$. *If the dimension of* $N_l(\mathbf{W}_{m\times m})$, *denoted as* $\dim N_l(\mathbf{W}_{m\times m})$, *is of* $(r+1)$, *then the LLE must be our linear mapping*.

Proof. Since the row-orthogonal matrix $\begin{bmatrix}\mathbf{V}_{r\times m} \\ (1/\sqrt{m})\mathbf{1}_m^{\mathrm{T}}\end{bmatrix}$ satisfies

$$\begin{bmatrix}\mathbf{V}_{r\times m} \\ \left(1/\sqrt{m}\right)\mathbf{1}_m^{\mathrm{T}}\end{bmatrix}\mathbf{W}_{m\times m} = \mathbf{0}_{(r+1)\times m}, \tag{11}$$

by $\dim N_l(\mathbf{W}_{m\times m}) = r+1$, each one of the row vectors of lower-dimensional data matrix $\mathbf{Y}_{d\times m}$ obtained by the LLE must be a linear combination of the row vectors of matrix $\mathbf{V}_{d\times m}$:

$$\mathbf{y}^i = \sum_{j=1}^{r} p_{ji}\mathbf{v}^j, \quad i = 1, 2, \ldots, d.$$

Hence,

$$\mathbf{Y}_{d\times r} = \mathbf{P}_{d\times r}\mathbf{V}_{r\times m}, \tag{12}$$

where $\mathbf{P}_{d\times r} = [p_{ij}]$, which defines a linear mapping from the r-dimensional space to d-dimensional space.

[1] In the LLE, the equality $\mathbf{Z}_{n\times m}\mathbf{W}_{m\times m} = \mathbf{0}_{n\times m}$ is implied. Otherwise, minimizing $\|\mathbf{Y}_{d\times m}\mathbf{W}_{m\times m}\|_F^2$ is meaningless. This is because if the equality does not hold, the obtained $\mathbf{Y}_{d\times m}$ from the minimization is not the best one in terms of local linearity preserving.