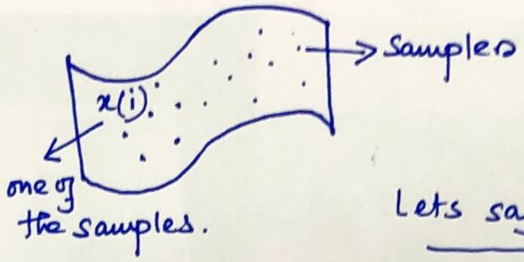
26.08.2024.

⇒ Locally linear Embedding: An unsupervised approach designed to transform data from its original high dimensional space to a lower-dimensional representation while considering non-linear structure.

- Saul, L.K., 'An Introduction to Locally Linear Embedding', (2000).
- Roweis, S.T., Saul, L.K., 'Non-linear dimensionality reduction by Locally linear Embedding', (2000), science, 290 (5500).




Many samples
- Each samples is a 'D' dimensional vector.

Lets say we have 'N' samples in the manifold.
& Each samples is a 'D' dimensional vector.

so, $x_i$ : $D \times 1$ vectors
$i = 1, 2, 3 \ldots N$

Define a parameter 'K'.
K defines the nearest neighborhood points of sample $x_i$
so in the example according to fig. drawn $K=5$.

In that case the o/p of LLE will be $Y(i)$: $M \times 1$ vectors.
so for 'N' no. of data points input dimensions 'D' is converted to output dimension 'M' where $M < D$.

<u>step ①</u> - <u>Local Linearization</u>

Define K-nearest neighborhood $N_i$ separately around each point $x_i$.

- Express $x(i)$ as the weighted sum of neighbors $x(j)$
- Minimize with respect to $\omega_{ij}$ : $\left\| x(i) - \sum_{j \in N_i} \omega_{ij}\, x(j) \right\|^2$

Hence $x(i) \approx \sum_{j \in N_i} \omega_{ij}\, x(j)$ $\quad x(i) \xrightarrow{\omega_{ij}} x(j)$

<u>step ②</u> - <u>Low Dimension Embedding</u>:

- Find $Y_i$ for all points
- Minimize with respect to $Y(i)$:

$$\sum_i \left\| Y(i) - \sum_{j \in N_i} \omega_{ij}\, Y(j) \right\|^2$$

Hence $Y(i) \approx \sum_{j \in N_i} \omega_{ij}\, Y(j)$ | $x(i) \xrightarrow{\omega_{ij}} x(j) \Rightarrow Y(i) \xrightarrow{\omega_{ij}} Y(j)$

⇒ Local Linearization:

- Given fix high-dim coordinates $x(i)$
- Find weights $w_{ij}$

- Express $x_i$ as the weighted sum of neighbors ~~of~~ $x(j)$

$$x(i) \approx \sum_{j \in N_i} w_{ij}\, x(j)$$

- weights $w_{ij}$ must satisfy : $\sum_{j \in N_i} w_{ij} = 1$.

- because :

<u>Translation Invariance</u>: Replace $x(i)$ with $x'(i) = x(i) - s$ then

$$x'(i) \approx \sum_{j \in N_i} w_{ij}\, x'(j)$$

<u>Rotation Invariance</u>: Replace $x(i)$ with $x'(i) = U x(i)$ then

$$x'(i) \approx \sum_{j \in N_i} w_{ij}\, x'(j)$$

$U$ = unitary $U$ is determined by the amount of rotation.

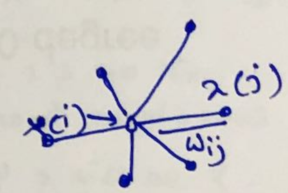
$x'(i) = x(i) - s$ then

$$\sum_{j \in N_i} w_{ij}\, x'(j) = \sum_{j \in N_i} w_{ij} \left[ x(j) - s \right]$$

$$= \sum_{j \in N_i} w_{ij}\, x(j) - \sum_{j \in N_j} w_{ij}\, s$$

$$\approx x_i - s = x'(i)$$

Now, Minimize : $\left\| x(i) - \sum_{j \in N_i} w_{ij}\, x(j) \right\|^2$ ;




$$= \left\| \sum_{j \in N_i} w_{ij} \left( x(i) - x(j) \right) \right\|^2$$

subject to $\left[ \sum_{j \in N_i} w_{ij} = 1 \right]$

if there are $k$ nearest neigbor for $x_i$ then

$$w_i = \begin{bmatrix} w_{i1} \\ w_{i2} \\ \vdots \\ w_{ik} \end{bmatrix} \quad (k \times 1) \quad \text{and} \quad w_i^T \mathbf{1} = 1.$$

Now consider the distance of these '$k$' nearest neighbors with respect to $x_i$

so, $z_i = \big[ \underbrace{x(1) - x(i) \;\ldots\; x(j) - x(i) \;\ldots\; x(k) - x(i)}_{} \big] \quad (D \times K)$

↓ all these are nothing but column of Matrix.

⇓ As you are dealing with '$D$' dimension with '$K$' nearest neigbbours so $D \times K$ Matrix.

So from $\left\| \sum_{j \in N_i} w_{ij} (x(j) - x(i)) \right\|^2$

will give none other than $\| z_i w_i \|^2 = (z_i w_i)^T (z_i w_i) = w_i^T z_i^T z_i w_i$
$= w_i^T G_i w_i$

where $G_i = z_i^T z_i$

Now previously $z_i$ was $D \times K$ dimension.

so $z_i^T$ will be $K \times D$

so $z_i^T . z_i$ will be a $K \times K$ Matrix.

so now, Minimize: $\omega_i^T G_i \omega_i$ so optimum $\omega_i = \frac{G_i^{-1} 1}{1^T G_i^{-1} 1}$

Subject to $\omega_i^T 1 = 1$.

- LLE Algorithm step 1: Input: $x(1) \ldots x(N)$

For each $x(i)$ do:

Find K-nearest neighborhood $N_i$ of $x(i)$

$z_i \leftarrow [\cdots (x_j - x_i) \cdots]$ [$z_i$ is all the nearest neighbors $- x_i$].

$G_i \leftarrow z_i^T z_i$

$\omega_i \leftarrow \frac{G_i^{-1} 1}{1^T G_i^{-1} 1}$

End

Now for Embedding i.e Low Dimensional Embedding $\omega_{ij}$ will be required.

find low-dimensional coordinates. $Y(i)$

Express $Y_i$ as weighted sum of neighbors $Y(j)$: $Y(i) \approx \sum_{j \in N_i} \omega_{ij} Y(j)$

Define weight Matrix $\omega$ $(N \times N)$ [N = no. of samples]

$$\omega_{ij} = \begin{cases} 0 & j = i \\ w_{ij} & j \in N_i \\ 0 & j \notin N_i \end{cases}$$

[$N_i$ stands for Neighborhood of $i$].

$$\begin{array}{cc} & \begin{array}{ccccccccc} & & & & & N_i & & & \end{array} \\ \text{row } i & \begin{bmatrix} \vdots & & & & & & & & \\ 0 & 0 & 0 & x & 0 & x & x & x & 0 \\ \vdots & & & & & & & & \end{bmatrix} \end{array}$$

these $x$'s are the K-nearest neighbours.

So no. of $x$ will be K.

all diagonal elements will be always '0' since $i = j$

- Define coordinate matrix $Y$ $(N \times M)$

$$Y = \begin{bmatrix} y^T(1) \\ \vdots \\ y^T(N) \end{bmatrix}$$