Locally Linear Embedding (LLE)
– To the memory of Sam Roweis (1972-2010)
Zengchang Qin (PhD)

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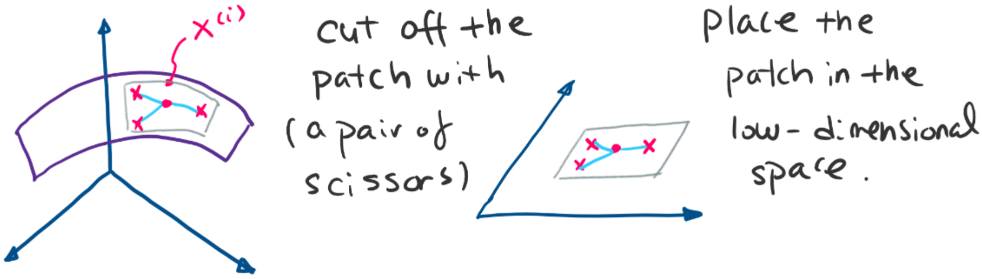
1) Consider a neighborhood of a manifold in a high-dimensional space R^n.



We hope to conserve the relations between the point and its neighbors.

2) $$\varepsilon^{(i)} = |x^{(i)} - \sum_j w^{(j)} \eta^{(j)}|^2$$
$$= |\Sigma_j w^{(j)} (x^{(i)} - \eta^{(j)})|^2$$

Since $\Sigma_j w^{(j)} = 1$, therefore,

$$\Sigma_j w^{(j)} (x^{(i)} - \eta^{(j)}) = \Sigma_j w^{(j)} x^{(i)} - w^{(j)} \eta^{(j)}$$
$$= x^{(i)} - \Sigma_j w^{(j)} \eta^{(j)}$$

Where $\eta^{(j)}$ for $j = 1, 2 \cdots k$ are the nearest neighbors of $x^{(i)}$, $x^{(i)} \in R^n$.

$$\varepsilon^{(i)} = |\Sigma_j w^{(j)} (x^{(i)} - \eta^{(j)})|^2$$
$$= \Sigma_j \Sigma_k w^{(j)} w^{(k)} C_{jk}$$

Where $C_{jk} = (x^{(i)} - \eta^{(j)}) \cdot (x^{(i)} - \eta^{(k)})$

$j, k = 1, 2 \cdots k$

In vector form ($Q = [(x^{(i)} - \eta^{(1)}), \cdots (x^{(i)} - \eta^{(k)})]^T$)

$$\varepsilon^{(i)} = \| Q W \|^2 = (Q W)^T (Q W)$$
$$= W^T Q^T Q W$$

The problem becomes a constrained square error minimization problem

$$\min_{W} \varepsilon^{(i)}$$
$$\text{s.t. } I^T W = 1 \quad (\textstyle\sum_j w^{(j)} = 1)$$

$$L = W^T Q^T Q W + \lambda (1 - I^T W)$$ Lagrangian multiplier

$$\frac{\partial L}{\partial W} = 0 \Rightarrow 2 Q^T Q W - \lambda I = 0$$
$$\Rightarrow W = \lambda I / 2 Q^T Q$$

Since $Q^T Q = C$

$$\Rightarrow W = \frac{\lambda}{2} C^{-1}$$

Because $I^T W = 1$

$$\Rightarrow W = \frac{\sum_j C_{jk}^{-1}}{\sum_p \sum_q C_{pq}^{-1}}$$

3) In the low-dimensional space, embedded vector y:

$$\min_{Y} \phi(Y) = \sum_{i=1}^{N} | y^{(i)} - \sum_{j=1}^{k} w^{(i,j)} y^{(j)} |^2$$

where $w^{(i,j)}$ is fixed from the original high-dimensional space.

By setting the following constraints:

$$\sum_i y^{(i)} = 0$$ Centered on 0

$$\frac{1}{N} \sum_i (y^{(i)} \cdot y^{(i)}) = I$$ 1 unit co-variance

Rewrite $\phi(Y)$ in vector form:

$$\phi(Y) = \Sigma_i | y^{(i)} - \sum_{j=1}^{k} w^{(j)} y^{(i,j)} |^2$$

$$= \Sigma_{i,j} M_{i,j} (y^{(i)} \cdot y^{(j)})$$

where $M = (I - W)^T (I - W)$

Given constraint $\Sigma_i y^{(i)} = 0$

$$L = M (y^{(i)} \cdot y^{(j)}) + \lambda \Sigma_i y^{(i)}$$

$$\frac{\partial L}{\partial y} = 0 \Rightarrow 2My = \lambda y$$

$$\Rightarrow My = \lambda y$$

By eigen decomposition, we can choose the eigen vectors with top a few eigen values.