

Computational Data Analysis

Machine Learning

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Associate Professor

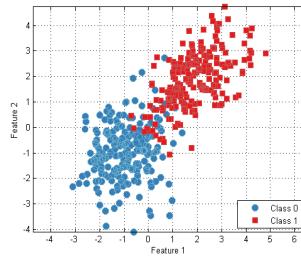
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Nonlinear Dimensionality Reduction

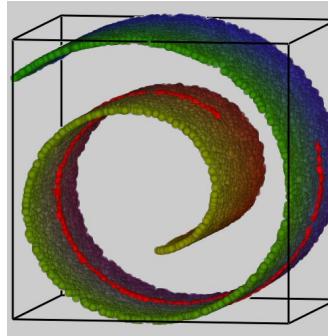
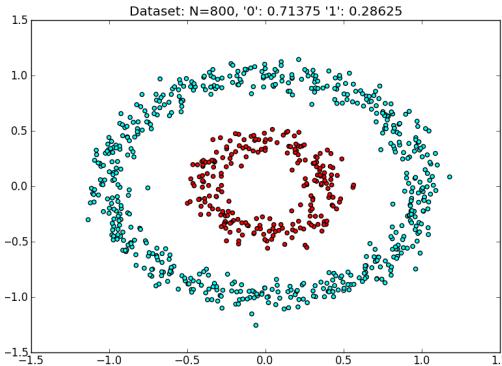


Limitation of PCA and SVD

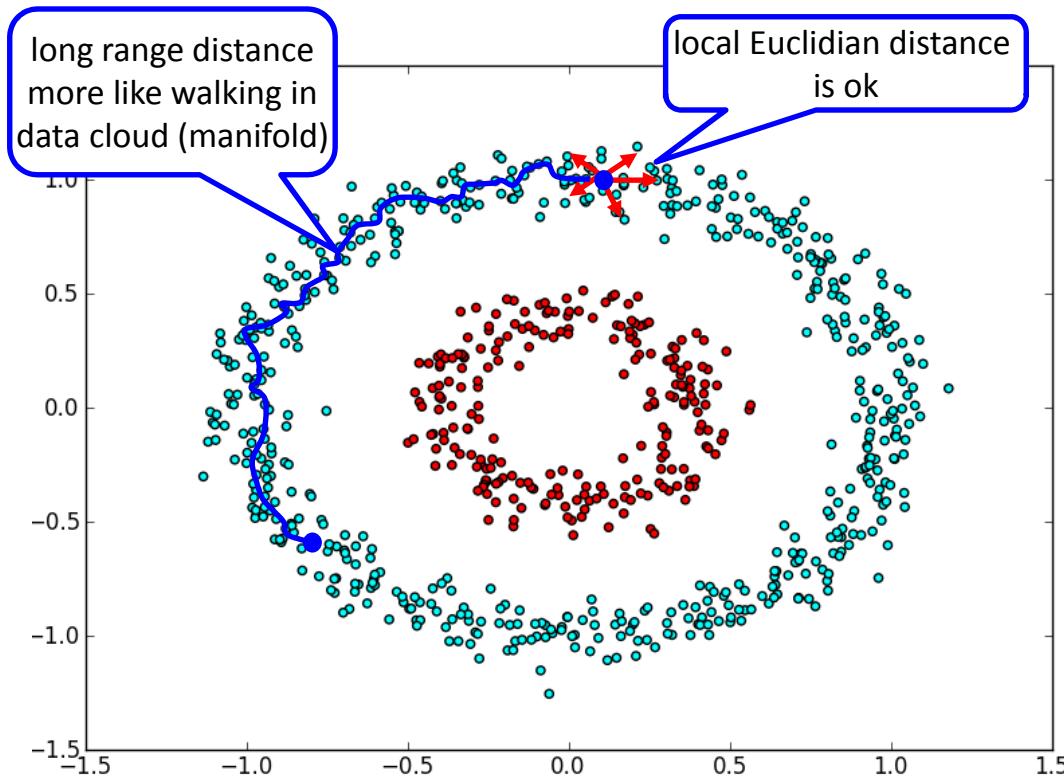
- Suitable when variables are linearly correlated



- Not suitable when nonlinear structures are present



What's a reasonable distance measure

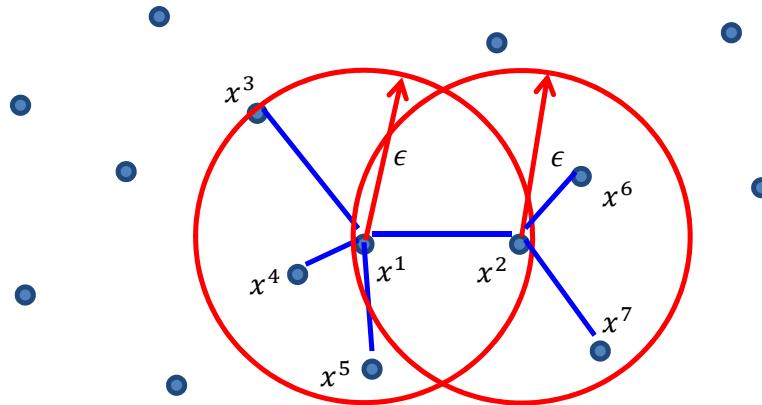


Recall: nearest neighbor graph

(c.f. spectral clustering)

- Given m data points, threshold ϵ , construct matrix $A \in R^{m \times m}$

$$A^{ij} = \begin{cases} 1, & \text{if } \|x^i - x^j\| \leq \epsilon \\ 0, & \text{otherwise} \end{cases}$$



Isomap

- Given m data points, $\{x^1, x^2, \dots, x^m\} \in R^n$
- Step 1: build a **weighted** graph A using nearest neighbors, and compute pairwise shortest distance matrix D

- Step 3: use a centering matrix $H = I - \frac{1}{m}11^\top$ to get

$$C = -\frac{1}{2m} H(D)^2 H$$

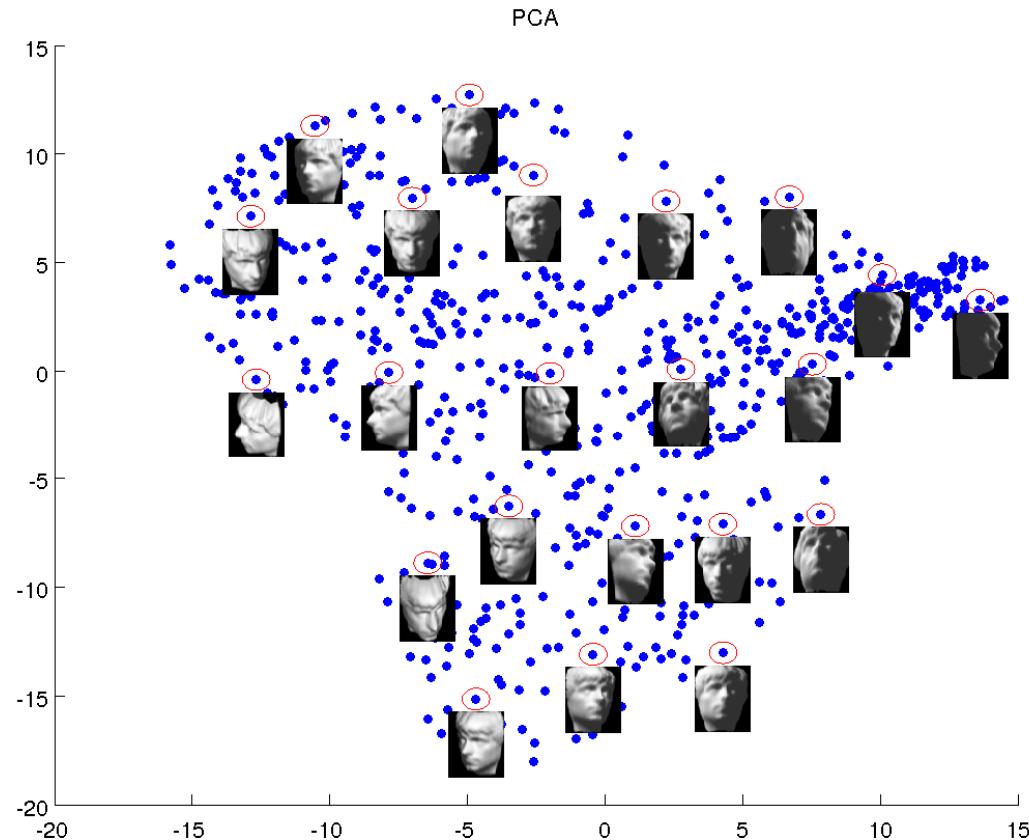
$$D_{ij}^2 := (D_{ij})^2$$

- Step 4: compute leading eigenvectors w^1, w^2, \dots and eigenvalues $\lambda_1, \lambda_2, \dots$ of C

$$Z^T = (w^1, w^2, \dots) \begin{pmatrix} \lambda_1^{1/2} & & \\ & \lambda_2^{1/2} & \\ & & \ddots \end{pmatrix}$$

Is the entrywise square of the distance matrix

Is the principal direction interpretable?



Result by isomap

