Spectral Embedding and Locally Linear Embedding

MUSTAFA HAJIJ

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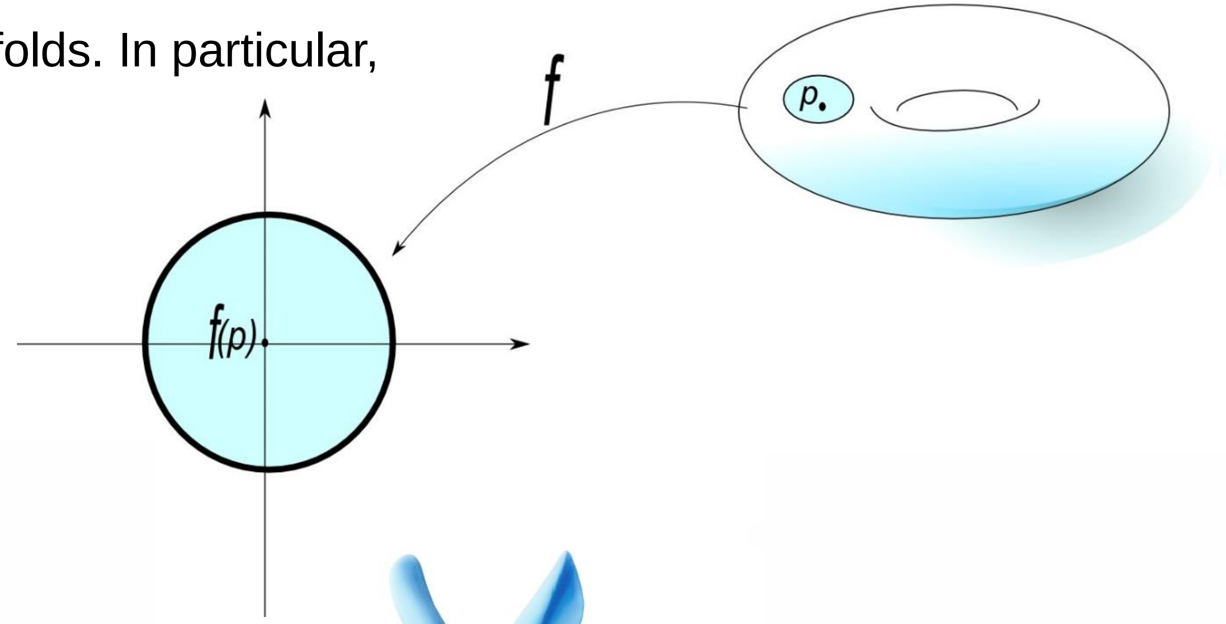

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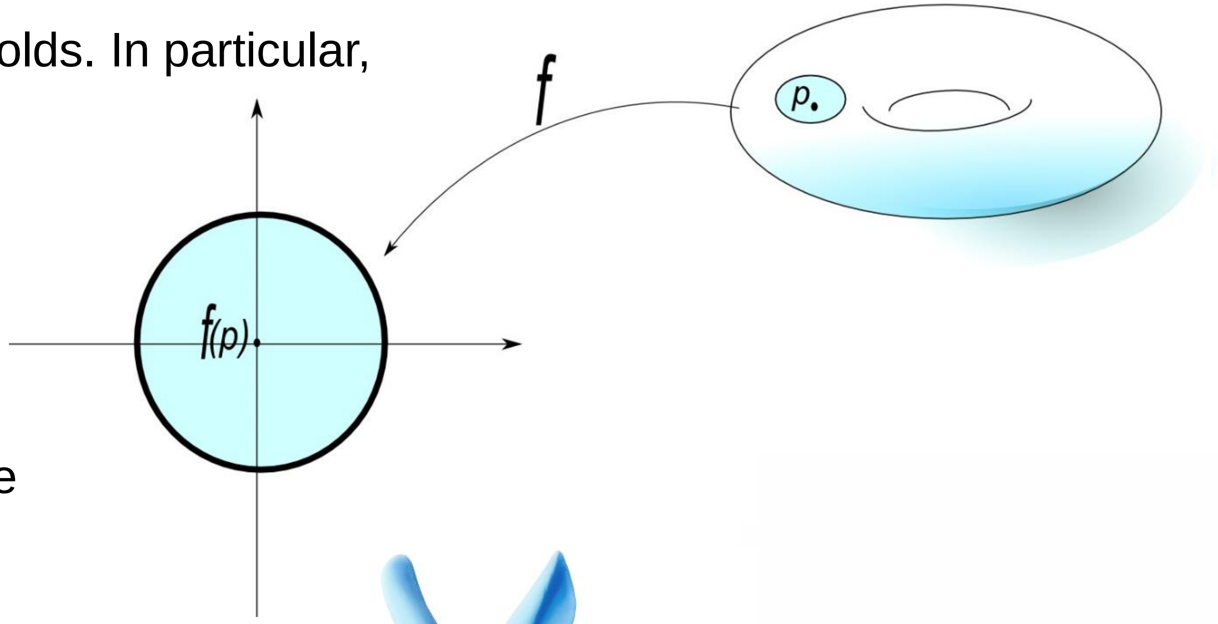

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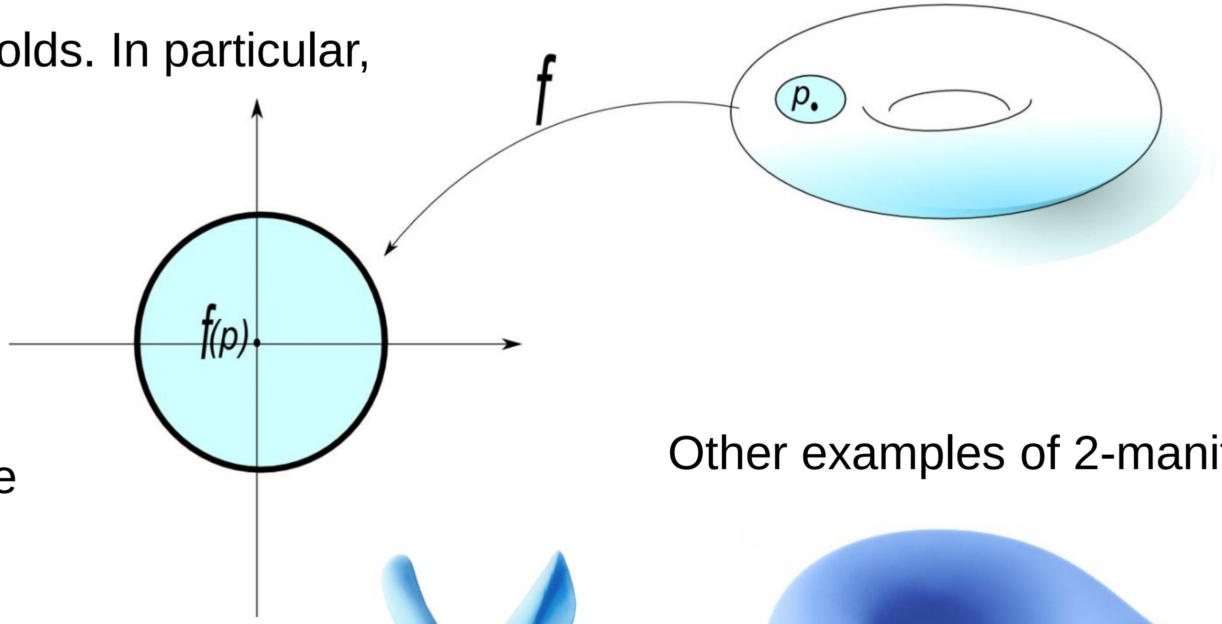

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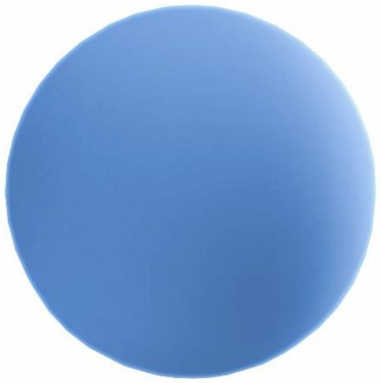
Other examples of 2-manifolds



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Locally linear embedding does not require the computation of the pair-wise distance matrix of the data such as ISOMAP and MDS.

LLE

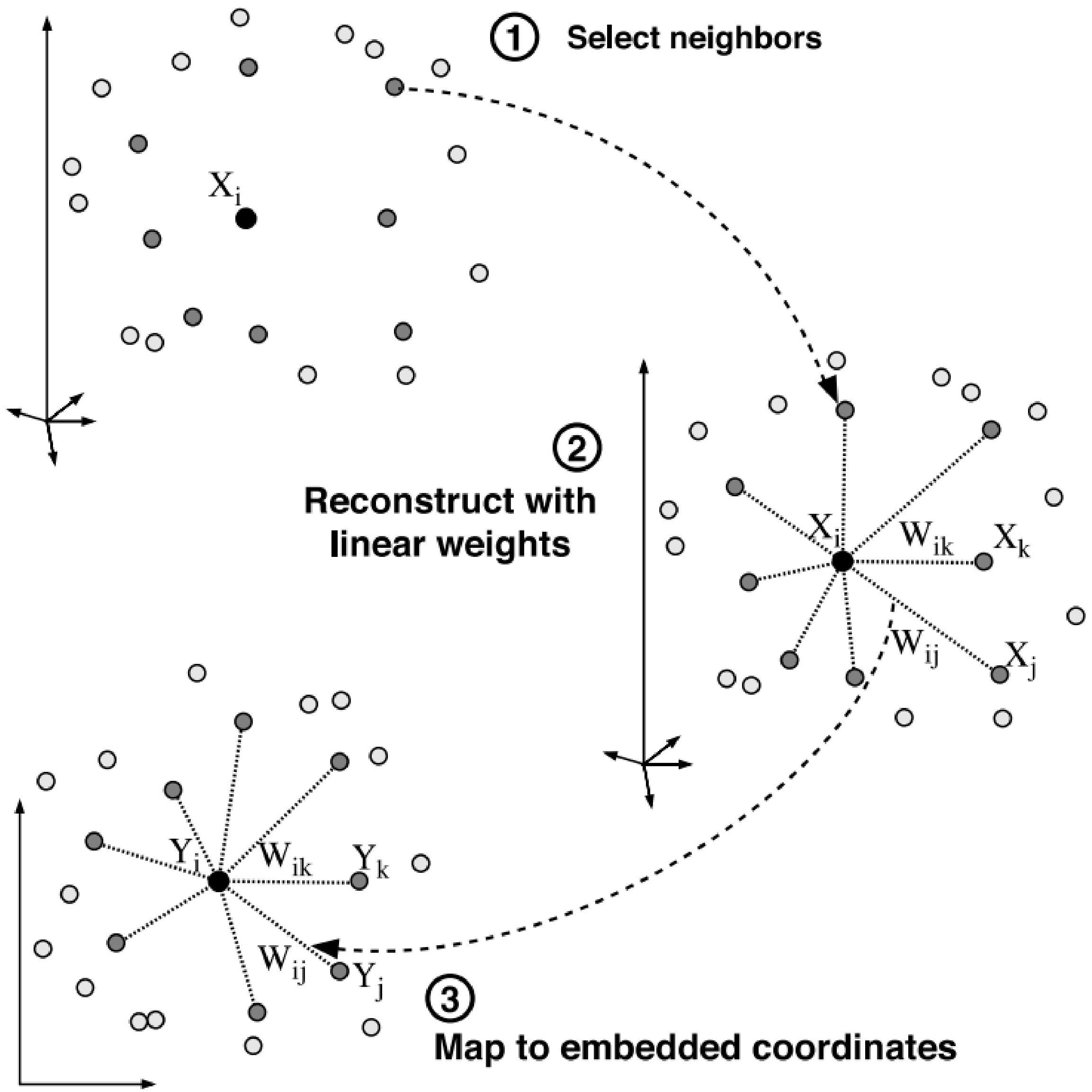


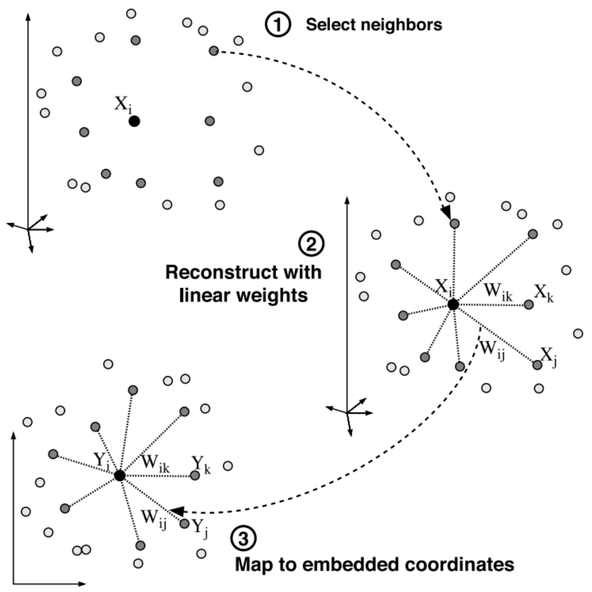
Image source, [original paper](#)

Basic idea

We need to optimize two objective functions in LLE :

I- $$\varepsilon(W) = \sum_i \left| \vec{X}_i - \Sigma_j W_{ij} \vec{X}_j \right|^2$$

Here we are given the points X_i and we are optimizing the weights W_{ij}



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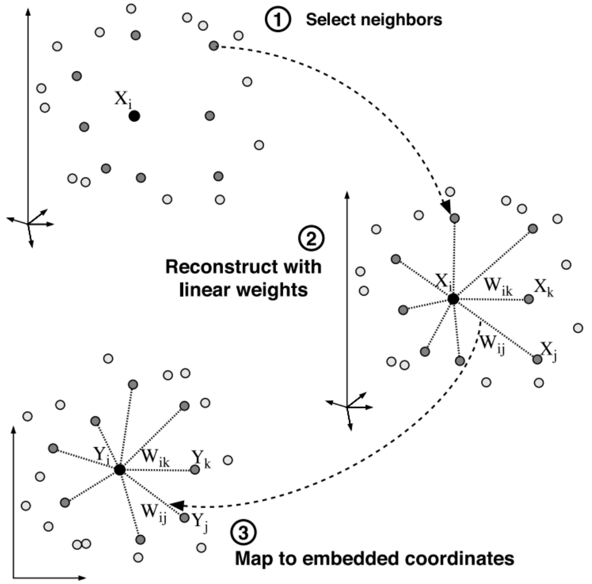
II- $$\Phi(Y) = \sum_i \left| \vec{Y}_i - \Sigma_j W_{ij} \vec{Y}_j \right|^2$$

Here we fix the weights W_{ij} while optimizing the coordinates Y_i



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Subject to the constrains :

(a) Wij=0 when Xj does not belong to the set of neighbors of Xi;

(b) $\sum_{j=1}^{k} W_{ij} = 1$

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Define $V_i = [X_{i(1)} X_{i(2)} \quad \ldots X_{i(k)}]$

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$$[X_i \ \ X_i \ldots X_i] = X_i e^T \text{ where } \quad e^T = [1, \ldots, 1]_{1*k}$$

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$The\ matrix\ G$ is called the Gram matrix

Details

Hence, write the objective function:

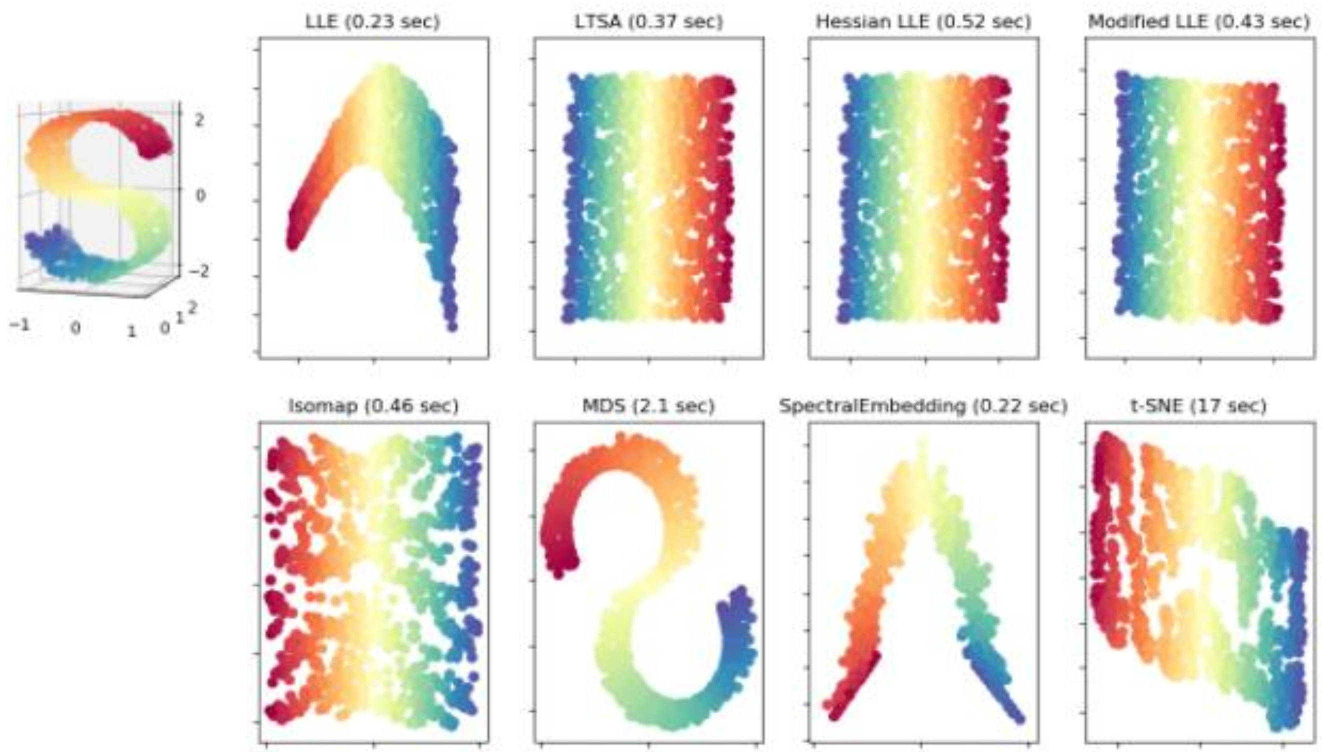
$$min \sum_{i} W_i^T G \mathrm{W_i}$$

Subject to $\sum_{j=1}^{k} W_{ij} = 1$

This is a well-known optimization problem and it can be solved using least square methods

LLE and its variation in Sklearn

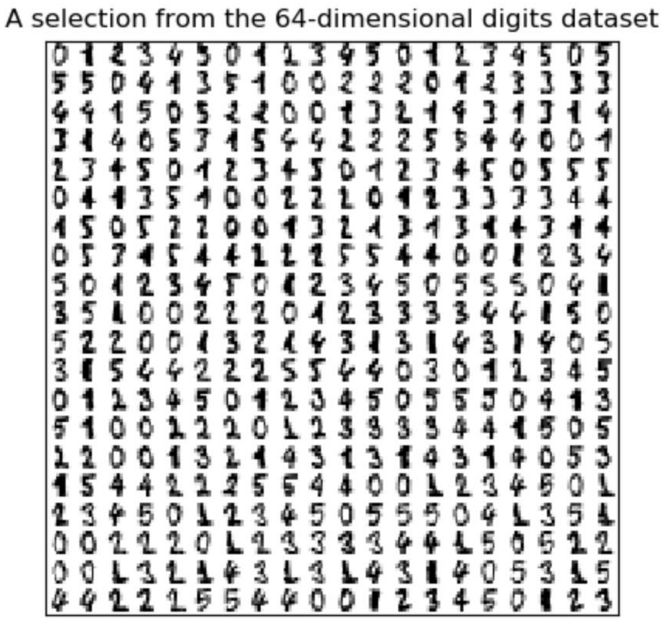
MDS is implemented in [Sklearn]



[Example]

Part II : Spectral Embedding

Spectral Embedding :example



spectral embedding

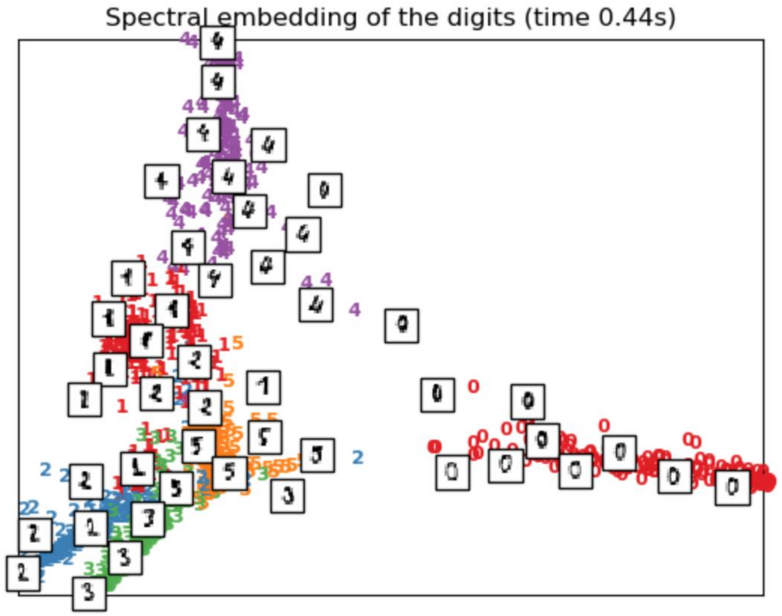


Image source: sklearn example

- The spectral embedding can unfold the nonlinear structures in a data in a high-dimensional feature space so that they become much easier to handle and understand.

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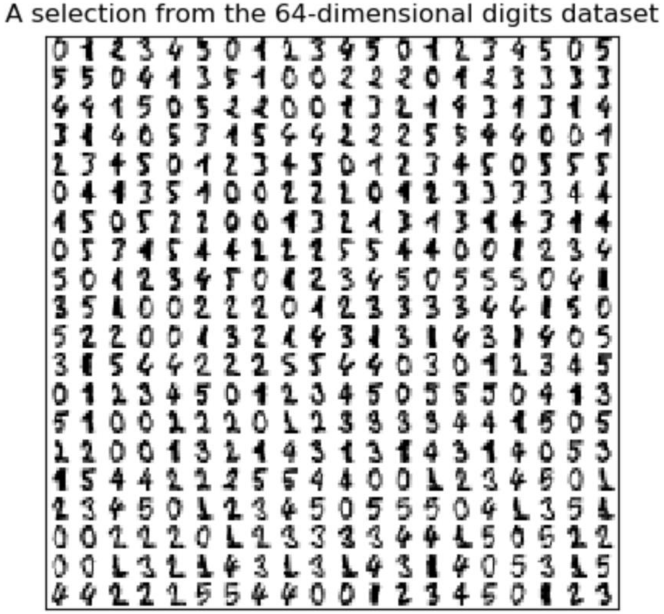

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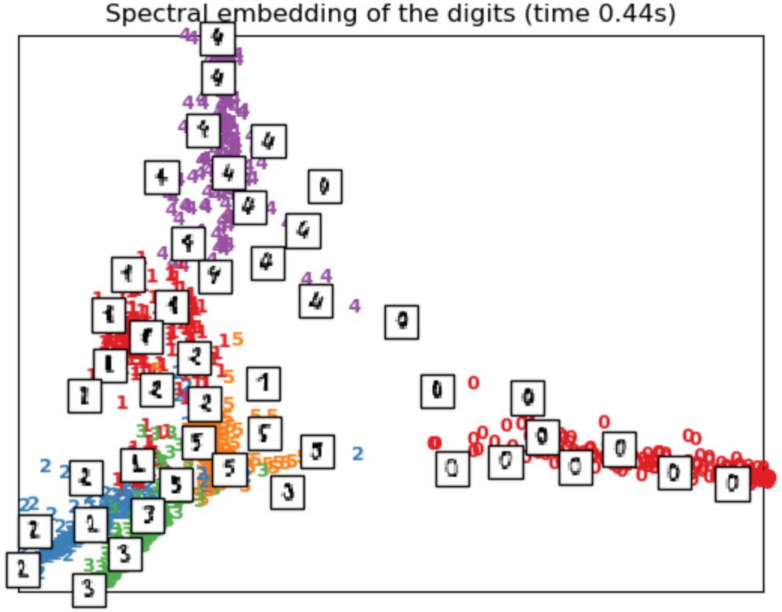

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spectral embedding

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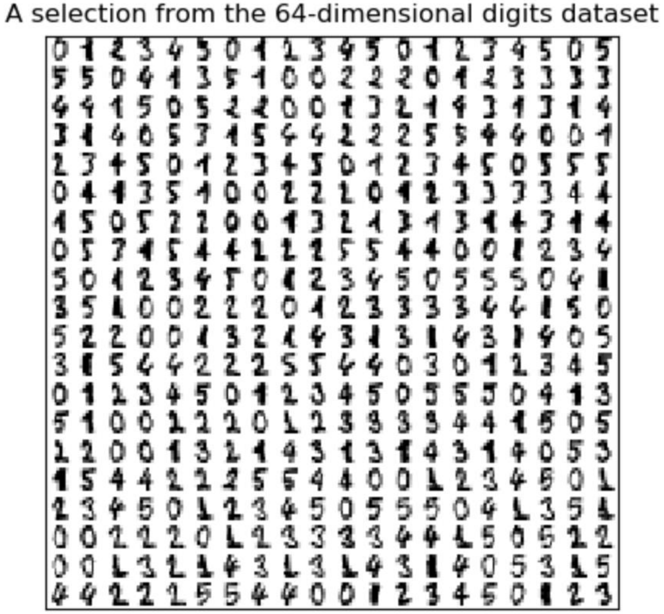

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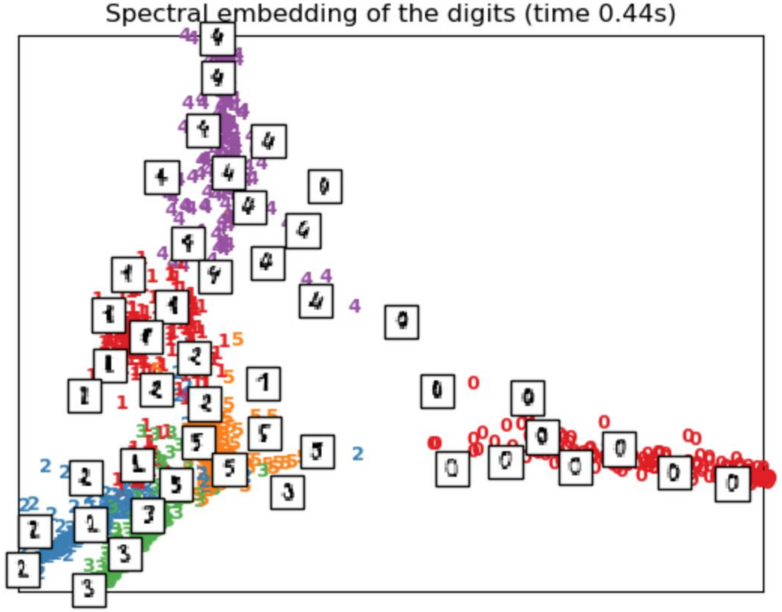

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Consider the digit dataset. This dataset can be thought of as a high-dimensional data with $d = 64$.

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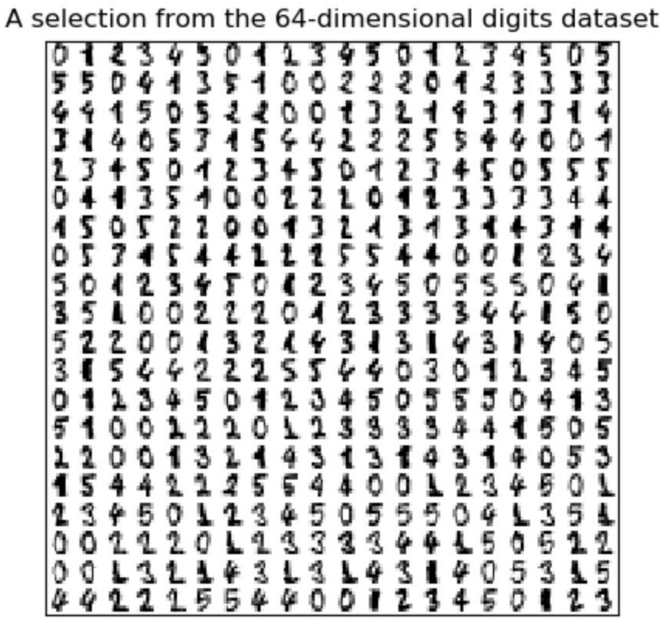

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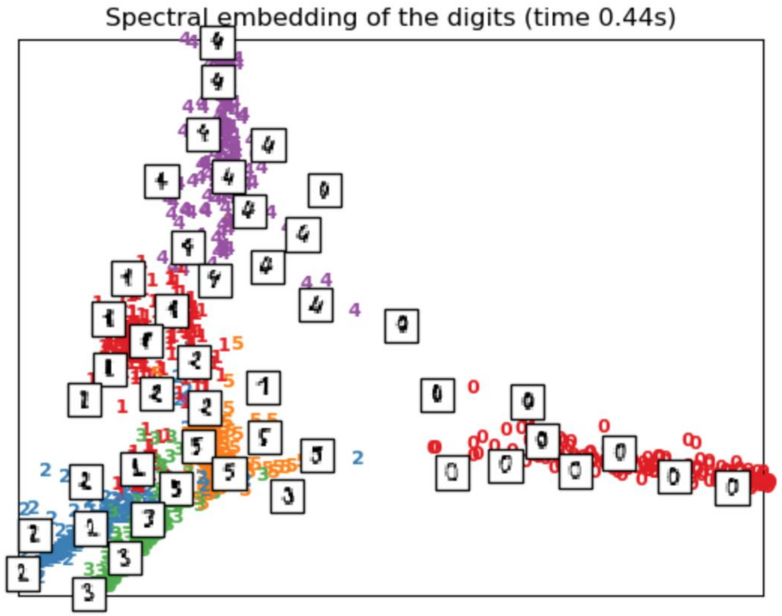

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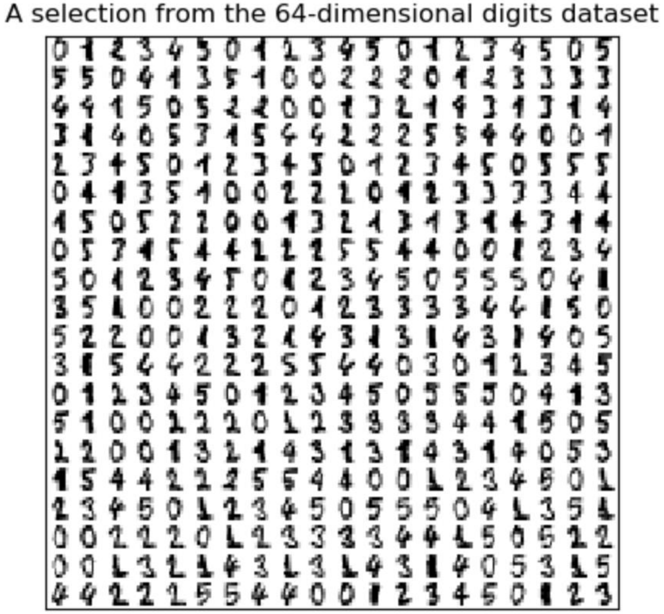

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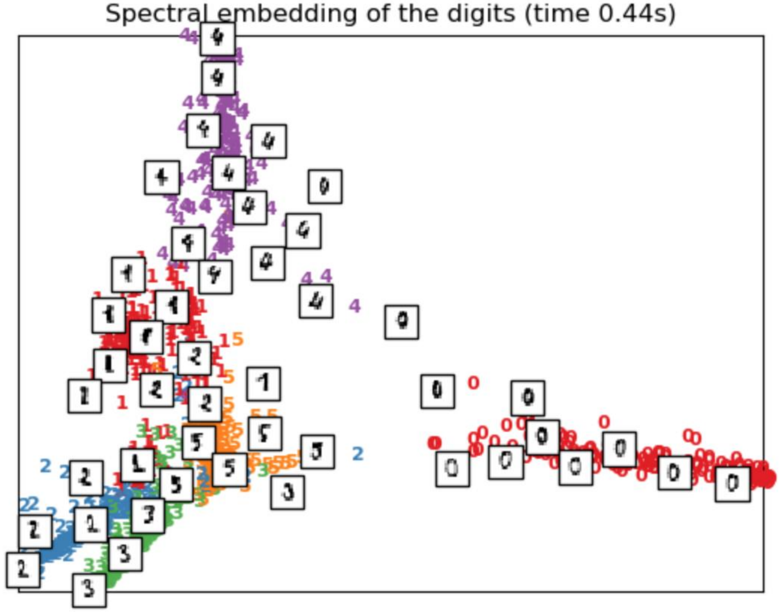

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In the example above we choose $k = 2$.

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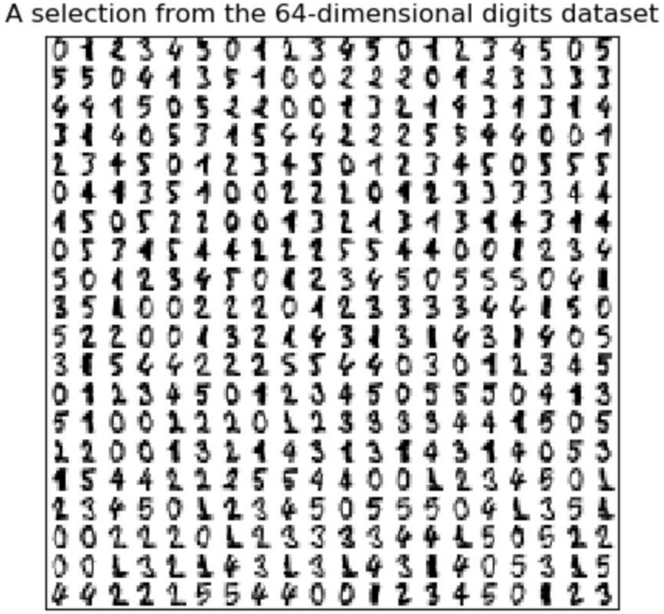

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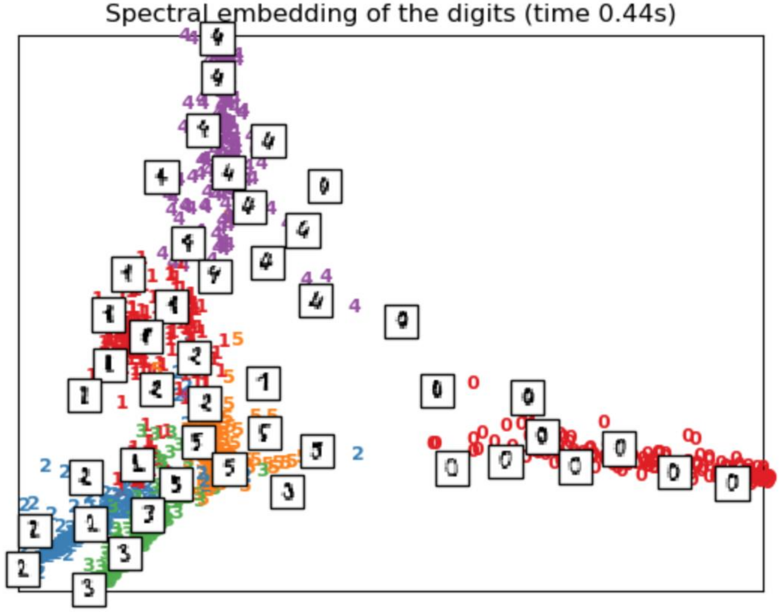

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But how exactly do we construct this new vector w ?

Spectral Embedding : general steps

- Construct a similarity graph phase : A similarity graph for the data X is chosen from the many available neighborhood graphs we studied in earlier lectures.
- The spectral embedding phase :In this step we use the eigenvectors of the Laplacian of the similarity graph to construct new coordinates.

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$$V=[v_1, v_2, \ldots, v_k]$$

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- Form W from V by normalizing the rows of W (making every row a unit vector).

Eigenvectors

V=$[v_1, v_2, \ldots, v_k]$

Column vectors

$$v_{ij} = \frac{u_{ij}}{\left(\sum_{l=1}^{k} u_{il}^2\right)^2}$$

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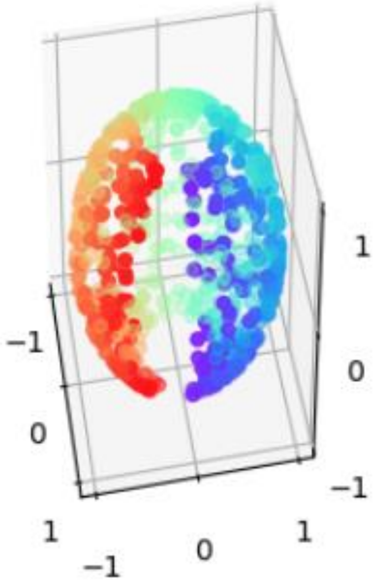
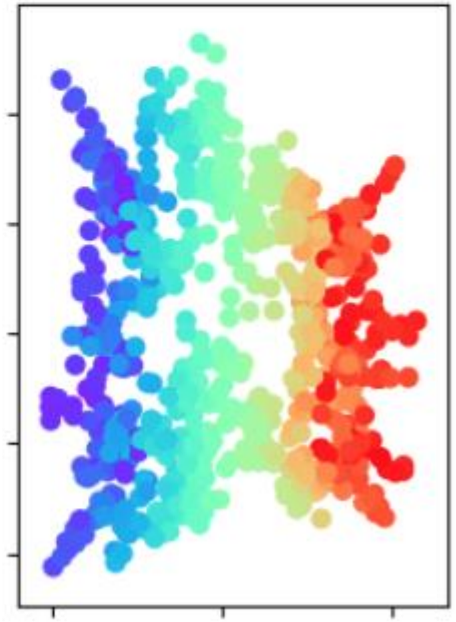
- Each row w_i in the matrix W is, by definition, the spectral embedding of the point x_i from the original data

Spectral Embedding :more examples



spectral embedding



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w=[w1,w2]

Image source: sklearn example

In general the results of spectral embedding can better reveal or exaggerate useful underlying structures in the input data.

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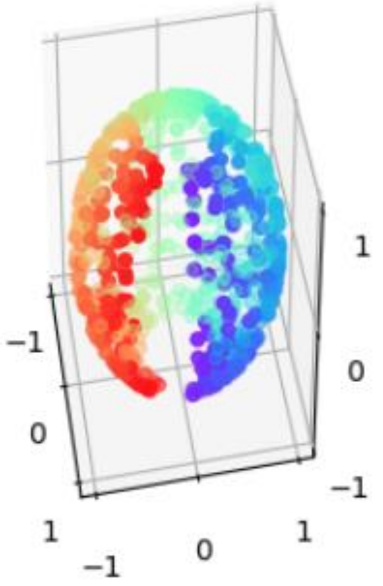

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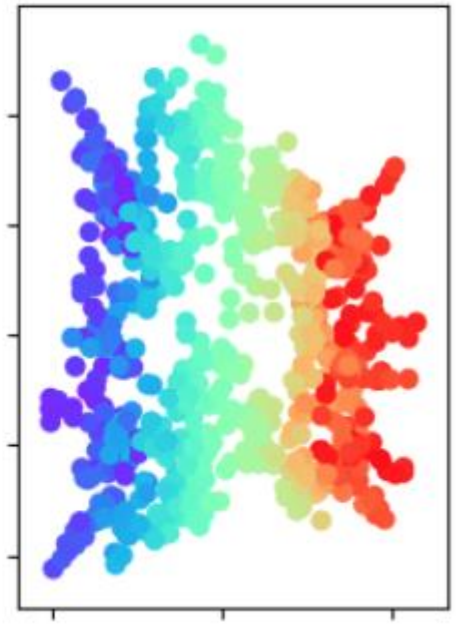

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Spectral embedding usually put the points that are highly similar closer to each other and the points that are dissimilar far away from each other

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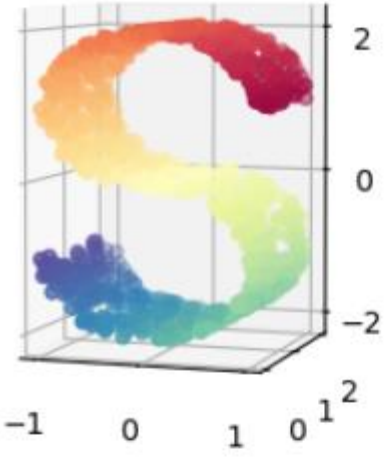

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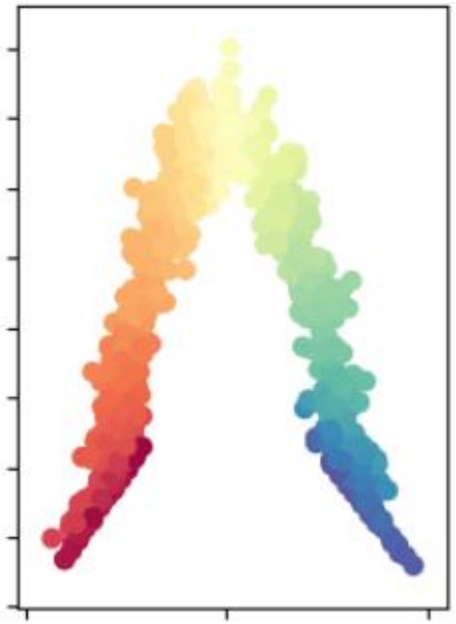

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Spectral Embedding :graphs

We can use spectral embedding to give an embedding for a graph.

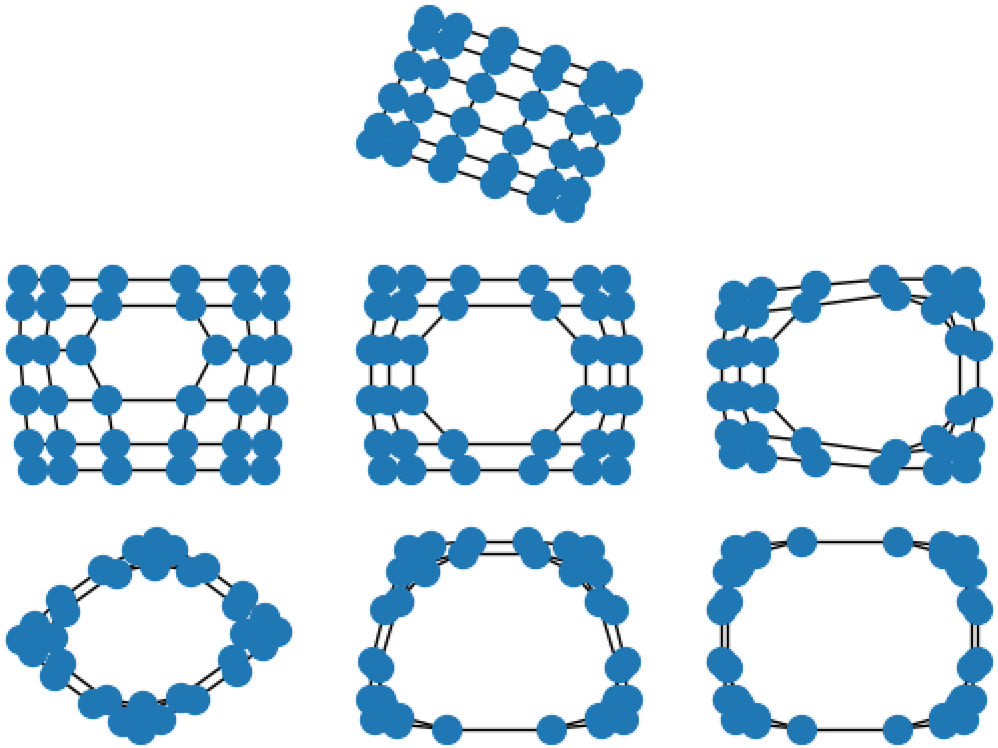

Image source:
networks example