ISOMAP

Similar to PCA, Metric Multidimensional Scaling (MDS) has been recently extended to perform nonlinear dimensionality reduction. A recent approach to nonlinear dimensionality reduction based on MDS is the Isomap algorithm.

Isomap is a nonlinear generalization of classical MDS. The main idea is to perform MDS, not in the input space, but in the geodesic (denoting the shortest possible line between two points on a sphere) space of the nonlinear data manifold. The geodesic distances represent the shortest paths along the curved surface of the manifold measured as if the surface were flat. This can be approximated by a sequence of short steps between neighbouring sample points. Isomap then applies MDS to the geodesic rather than straight line distances to find a low-dimensional mapping that preserves these pairwise distances

The Isomap algorithm proceeds in three steps:

1. Find the neighbours of each data point in high-dimensional data space.
2. Compute the geodesic pairwise distances between all points.
3. Embed the data via MDS so as to preserve these distances.

The first step can be performed by identifying the k nearest neighbours, or by choosing all points within some fixed radius, ϵ. These neighbourhood relations are represented by a graph G in which each data point is connected to its nearest neighbours, with edges of weight d_X(i, j) between neighbours.

The geodesic distances d_M(i, j) between all pairs of points on the manifold M are then estimated in the second step. Isomap approximates d_M(i, j) as the shortest path distance d_G(i, j) in the graph G. This can be done in different ways including Dijkstra's algorithm and Floyd's algorithm.

These algorithms find matrix of graph distances $D^{(G)}$ contains the shortest path distance between all pairs of points in G. In its final step, Isomap applies classical MDS to $D^{(G)}$ to generate an embedding of the data in a d-dimensional Euclidean space Y. The global minimum of the cost function is obtained by setting the coordinates of y_i to the top d eigenvectors of the inner-product matrix B obtaines from $D^{(G)}$.

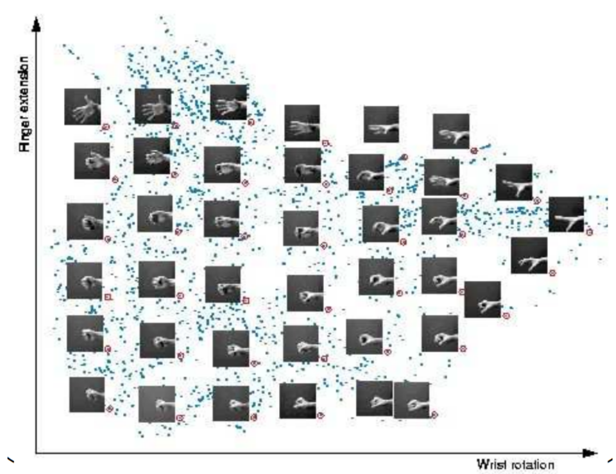

Figure 1: Hand position example

For example, Isomap (K=6) applied to N=2000 images (64 pixels by 64 pixels) of a hand in different configurations. The images were generated by making a series of opening and closing movements of the hand at different wrist orientations, designed to give rise to a two-dimensional manifold. The images were treated as 4096-dimensional vectors, with input-space distances defines in the Euclidean metric. Isomap correctly detects two clearly significant dimensions, plus several weak dimensions of noise; PCA and MDS do not detect the correct dimensionality and suggest a much higher level of noise. The recovered coordinate axes map approximately onto the distinct underlying degree of freedom: wrist rotation (x-axis) and finger extension (y-axis).

Locally Linear Embedding

Locally linear embedding (LLE) is another approach which address the problem of nonlinear dimensionality reduction by computing low-dimensional, neighbourhood preserving embedding of high-dimensional data. A data set of dimensionality n, which is assumed to lie on or near a smooth nonlinear manifold of dimensionality d <n, is mapped into a single global coordinate system of lower dimensionality, d. The global nonlinear structure is recovered by locally linear fits. Consider t n-dimensional real-valued vectors x_i sampled from some underlying manifold. We can assume each data point and its neighbours lie on, or are close to, a locally linear patch of the manifold.

By a linear mapping, consisting of a translation, rotation, and rescaling, the high-dimensional coordinates of each neighbourhood can be mapped to global internal coordinates on the manifold. Thus, the nonlinear structure of the data can be identified through two linear steps: first, compute the locally linear patches, and second, compute the linear mapping to the coordinate system on the manifold.

The main goal here is to map the high-dimensional data points to the single global coordinate system of the manifold such that the relationships between neighbouring points are preserved.

References

Manifold Learning Examples http://axon.cs.byu.edu/Dan/678/miscellaneous/Manifold.example.pdf

Manifold Learning and it's application https://www.cse.iitk.ac.in/users/se367/10/se367.pdf