Isometric Feature Mapping (ISOMAP)

Additional reading can be found from non-assessed exercises (week 10) in this course unit teaching page. Textbook: Sect. 6.7 in [1]
Outline

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Introduction

- Isometric feature mapping (ISOMAP)
  - A state-of-the-art non-linear MDS method for modelling manifold structure appearing in a high dimensional space
  - In ISOMAP, a geodesic distance metric is employed.
  - Useful for recovering a low dimensional isometric embedding
Basics of Non-Euclidian Space

Metric model

Shape = metric space $(X, d)$
Similarity = isometry w.r.t. $d$

EXTRINSIC GEOMETRY

- Euclidean metric $d_{\mathbb{R}^3}|_X$
- Invariant to rigid motion

Extrinsic geometry is not invariant under inelastic deformations
Basics of Non-Euclidian Space

Metric model

- Shape = metric space $(X, d)$
- Similarity = isometry w.r.t. $d$

EXTRINSIC GEOMETRY
- Euclidean metric $d_{\mathbb{R}^3}|_X$
- Invariant to rigid motion

INTRINSIC GEOMETRY
- Geodesic metric $d_X$
- Invariant to inelastic deformation
Basics of Non-Euclidian Space

Isometric embedding

\[ d_X(x_1, x_2) = d_{\mathbb{R}^3}(\varphi(x_1), \varphi(x_2)) \]
**ISOMAP Algorithm**

- **One possible solution (ISOMAP)**
  - To find the embedding manifold, find a transformation that preserves the **geodesic** distances between points in the high-dimensional space
    - This approach is related to multidimensional scaling (e.g., Sammon’s mapping; **MDS slides**), except for MDS seeks to preserve the **Euclidean** distance in the high-dimensional space
  - The issue becomes how to compute geodesic distances from sample data
ISOMAP Algorithm

- **ISOMAP** [Tenenbaum et al., 2000] is based on two simple ideas
  - For neighboring samples, Euclidean distance provides a good approximation to geodesic distance
  - For distant points, geodesic distance can be approximated with a sequence of steps between clusters of neighboring points

- **ISOMAP operates in three steps**
  - Find nearest neighbors to each sample
  - Find shortest paths (e.g., Dijkstra)
  - Apply MDS
ISOMAP Algorithm

**STEP 1**

- Determine which points are neighbors in the manifold, based on the distances $d_X(i,j)$ in the input space $X$.
- This can be performed in two different ways:
  - Connect each point to all points within a fixed radius $\varepsilon$.
  - Connect each point to all of its $K$ nearest neighbors.
- These neighborhood relations are represented as a weighted graph $G$, each edge of weight $d_X(i,j)$ between neighboring points.
- Result:
ISOMAP Algorithm

**STEP 2**
- Estimate the geodesic distances $d_M(i,j)$ between all pair of points on the manifold $M$ by computing their shortest path distances $d_G(i,j)$ in the graph $G$
- This can be performed, e.g., using Dijkstra’s Algorithm

**STEP 3**
- Find $d$-dim embedding $Y$ that best preserves the manifold’s estimated distances
  - In other words, apply classical MDS to the matrix of graph distances $D_G = \{d_G(i,j)\}$
  - The coordinate vectors $y_i$ are chosen to minimize the following cost function
    \[
    E = \| \tau(D_G) - \tau(D_Y) \|_2
    \]
    where $D_Y$ denotes the matrix of Euclidean distances $\{d_Y(i,j)=\|y_i - y_j\|\}$, and operator $\tau$ converts distances to inner products
    \[
    \tau(S) = -HSH/2
    \]
    where $S$ is the matrix of squared distances $\{S_{ij}=D^2_{ij}\}$, and $H$ is a centering matrix, defined as
    \[
    H = I - \frac{1}{N} ee^T; \quad e = [1\ 1\ldots 1]^T
    \]
  - It can be shown that the global minimum of $E$ is obtained by setting the coordinates $y_i$ to the top $d$ eigenvectors of the matrix $\tau(D_G)$
ISOMAP Algorithm

1. **Construct neighborhood graph**
   (a) Define graph $G$ by connecting points $i$ and $j$ if they are [as measured by $d_x(i,j)$] closer than epsilon (epsilon - Isomap), or if $i$ is one of the $K$ nearest neighbors of $j$ (K-Isomap).
   (b) Set edge lengths equal to $d_x(i,j)$.

2. **Compute shortest paths**
   (a) Initialize
   $d_G(i,j) = d_x(i,j)$ if $i,j$ are linked by an edge;
   $d_G(i,j) = \infty$ otherwise.
   (b) For $k = 1, 2, ..., N$, replace all entries $d_G(i,j)$ by $\min\{d_G(i,j), d_G(i,k) + d_G(k,j)\}$.
   (c) Matrix $D_G = \{d_G(i,j)\}$ will contain the shortest path distances between all pairs of points in $G$.

3. **Construct d-dimensional embedding**
   (a) Let $\lambda_p$ be the $p$-th eigenvalue (in decreasing order) of the matrix $\tau(D_G)$, and $v_p^i$ be the $i$-th component of the $p$-th eigenvector.
   (b) Set the $p$-th component of the $d$-dimensional coordinate vector $y_i$ equal to $\sqrt{\lambda_p}v_p^i$. 
Fig. 3. The “Swiss roll” data set, illustrating how Isomap exploits geodesic paths for nonlinear dimensionality reduction. (A) For two arbitrary points (circled) on a nonlinear manifold, their Euclidean distance in the high-dimensional input space (length of dashed line) may not accurately reflect their intrinsic similarity, as measured by geodesic distance along the low-dimensional manifold (length of solid curve). (B) The neighborhood graph $G$ constructed in step one of Isomap (with $K = 7$ and $N = 1000$ data points) allows an approximation (red segments) to the true geodesic path to be computed efficiently in step two, as the shortest path in $G$. (C) The two-dimensional embedding recovered by Isomap in step three, which best preserves the shortest path distances in the neighborhood graph (overlaid). Straight lines in the embedding (blue) now represent simpler and cleaner approximations to the true geodesic paths than do the corresponding graph paths (red).
Example

N = 1000
\( \varepsilon = 4.2 \)
Relevant Issues

■ ISOMAP is guaranteed asymptotically to recover the true dimensionality and geometric structure of a certain class of Euclidean manifolds
  • These are manifolds whose intrinsic geometry is that of a convex region of Euclidean space, but whose geometry in the high-dimensional space may be highly folded, twisted or curved
    ■ Intuitively, in 2D, these include any physical transformations one can perform on a sheet of paper without introducing tears, holes, or self-intersections
  • For non-Euclidean manifolds (hemispheres or tori), ISOMAP will still provide a globally-optimal low-dimensional representation

■ Mapping
  • Note that ISOMAP does not provide a mapping function $Y = f(X)$
  • One could however be learned from the pairs $\{X_i, Y_i\}$ in a supervised fashion

out-of-sample extension
Conclusions

- ISOMAP is a nonlinear MDS method to recovering intrinsic manifold in a low dimensional space via minimum distortion embedding.
- It has three steps: a) construct a neighbourhood graph, b) compute shortest path and c) construct low-dimensional embedding.
- ISOMAP can fail in its two main steps:
  - Geodesic Approximation
    - Points need to be sampled uniformly (densely) from a noiseless manifold.
    - The intrinsic parameter space must be convex.
  - MDS
    - There might not exist an isometric embedding
- Suffer from a high computational cost and sensitive to noise.
- There are several extensions to overcome those problems.