COMPSCI 589
Lecture 22: Multidimensional Scaling and Isomap

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Created with support from National Science Foundation Award# IIS-1350522.

Outline

1. Review
2. MDS
3. Isomap

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- We showed that basis expansion can be combined with PCA and SVD, but that PCA could also be used with the kernel trick.
- Lastly, we saw how spectral clustering can be viewed as a modification of clustering in the kernel PCA latent space.

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- Suppose we have a data set $\mathcal{D} = \{\mathbf{x}_i \in \mathbb{R}^D\}_{i=1:N}$.
- Let d_{ij} be the distance between $\mathbf{x}_i$ and $\mathbf{x}_j$. Any distance metric can be used. Euclidean distance $d_{ij} = ||\mathbf{x}_i - \mathbf{x}_j||$ is common.

Least Squares Multidimensional Scaling

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- Basically, this function attempts to have the regular Euclidean distances between points in $\mathbb{R}^K$ reflect the distances between the points in $\mathbb{R}^D$. This can be useful for data visualization when $K = 2$.

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- If the similarities are centered inner products in $\mathbb{R}^D$, Classical MDS and PCA are equivalent. For other similarity functions, classical MDS performs non-linear dimensionality reduction.

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MDS Trade-offs

- Interestingly, to use MDS we actually don't need the raw feature vectors. It's enough to have the pairwise distance or similarity matrices.
- Unlike kernel PCA, the similarity or distance matrices do not need to be valid kernel matrices (ie: they do not need to correspond to inner products of some basis expansion).
- A significant issue with MDS is that we need to be able to specify a global similarity or distance matrix directly. This may not actually be easy to do if the data come from a complex manifold (regular Euclidean distance will fail).

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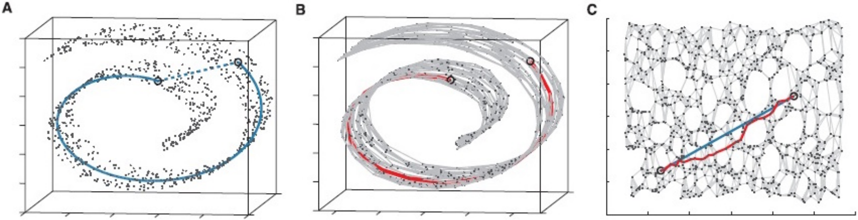

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- For points i, j that are not neighbors in the graph, isomap uses the length of the shortest path in G as d_{ij}. This is an approximation to the geodesic distance between $\mathbf{x}_i$ and $\mathbf{x}_j$ on the manifold.
- Finally, isomap plugs the distances d_{ij} into MDS with classical scaling and computes the embedding.