Improving LIBS Analysis using Non-linear Dimensionality Reduction

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Laser Induced Breakdown Spectroscopy (LIBS) - LIBS is a rapid chemical analysis technique that is used to analyze the spectrum for photon energy radiated by a compound. The compound is excited by a short laser pulse the compound then emits some energy that is collected and recorded.

1. Data Reduction

The compound's spectrum is composed of a large number of spectra lines resulting in a dataset that has a high dimensionality. The dimensionality of the data increases the complexity of uncovering patterns within the data because it makes it difficult to visualize the relationship among the dataset and detecting which spectra line is redundant. In reducing the data's dimensionality, care must be exercised not to compromise data-integrity by damaging important structure.

2. Manifold Learning

Manifold methods are class of techniques that include information about the geometry of the underlying surface along which data-points reside. This is accomplished by encoding the relationships among data-points within a given neighborhood. An important consideration concerns the size of the neighborhood. That is, how far away from each data-point should relationships be considered in order to properly encode geometry? With a good representation of geometry, a manifold method preserves relationships among data-points while facilitating compact dimension reduced representations

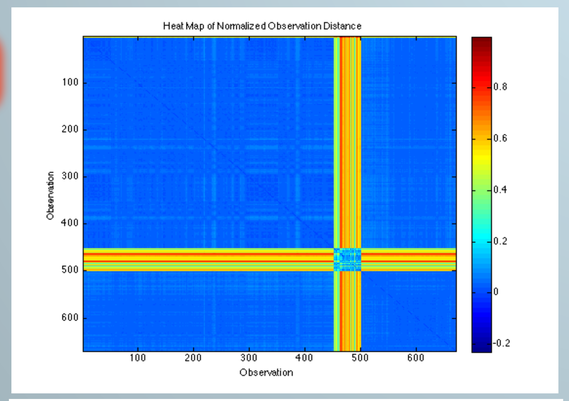
3. Algorithm

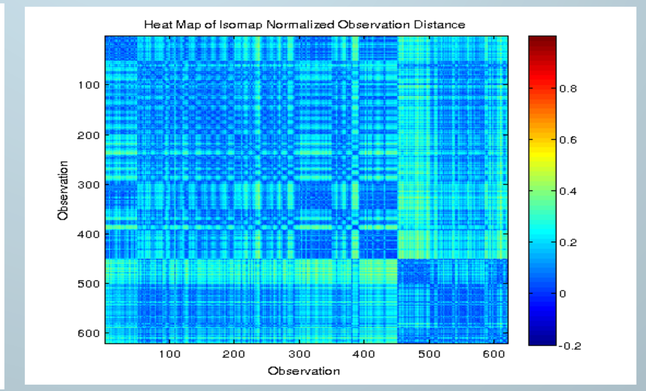
1) Load the LIBS data file
2) Preform dimension reduction
   - Create distance matrix from all possible pairs of observations
   - Create an Isometric Mapping manifold and figure out which neighborhood size provides the best representation
3) Create heat map

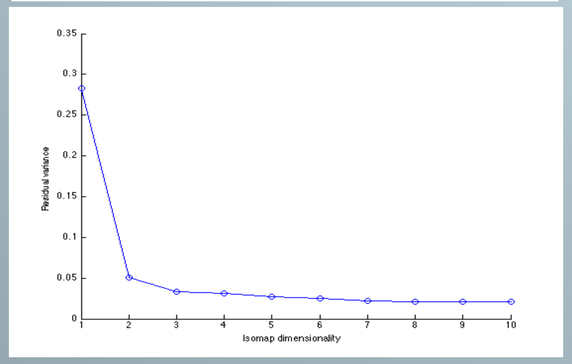
4. RESULTS

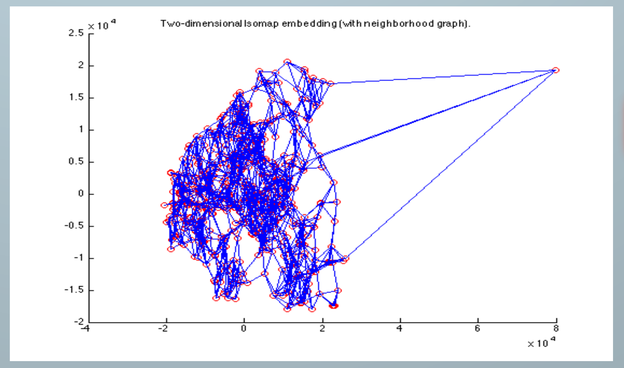
Heat Map

Observations	Amino
1 – 50	Water
51 – 100	ASP
101 – 150	Glu
151 – 200	Cys
201 – 250	Water
251 – 300	ASP
301 – 350	Glu
351 – 400	Cys
401 – 450	Polysaccharide
451 – 500	Ser D
501 – 550	Water
550 – 650	Water
650 – 670	Water









5. Conclusion and Future work

Manifolds preserves relationships among data-points while facilitating compact dimension reduced representations. In my work, I experiment with the effect of neighborhood size on representational power for a challenging LIBS data set. Applications of my research includes discovery of spectral patterns associated with protein configurations of cancer cells, possibly leading to improved detection.

6. ACKNOWLEDGEMENTS

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