Research Directions to Validate Topological Models of Multi-Dimensional Data

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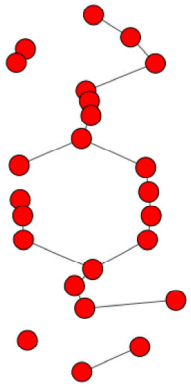
Goal

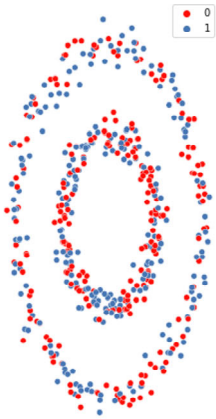
Topological methods in machine learning aim to quantitatively encode shape information from multi-dimensional data points.
Validation relies on defining a validation measure to compare topological models.

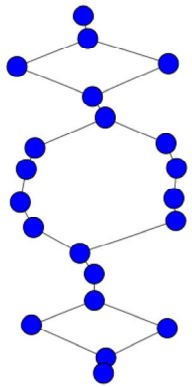
What could be a validation measure relating topological properties of the model and statistical properties of the data for the Mapper [1] and the Generative Simplicial Complex [2,3,4] models?

Research directions for validation

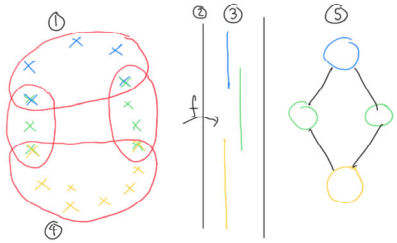
Different samples (blue/red) from the same distribution.
But very different Mapper nerves…





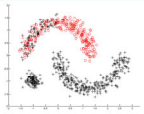


Mapper [1]



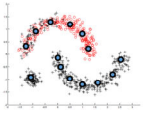
1) Input data
2) Filter function f
3) Cover $Im(f)$
4) Cluster preimages
5) Compute nerve

[2,3,4] Generative Simplicial Complex



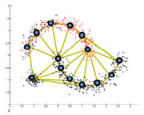
Input

1) Input (labeled) data $x \in \mathbb{X}$

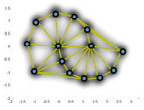


GSC

2) Gaussian Mixture Model
- Parameters θ estimated with Expectation Maximization (EM)
- #centers w selected with Bayesian Information Criterion (BIC)

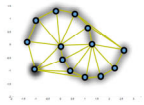


3) Delaunay complex of GMM centers w (Here the case of the Delaunay Graph)

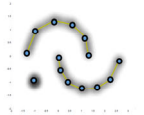


4) Gaussian kernel $g(x, w, \theta)$ convoluted to each simplex W_σ with its own prior weight π_σ

$$p(x, S, W, \theta) = \sum_{\sigma \in S} \frac{\pi_\sigma}{|W_\sigma|} \int_{W_\sigma} g(x, w, \theta) dw$$

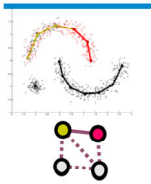


5) EM: prior weights of generative simplices which do not explain data tend towards 0



6) BIC: Simplices with 0 prior get pruned

Output



7) Max A Posteriori gives class label for each simplex

8) Summary graph/simplex based on connected components in initial and pruned Delaunay complex

References

[1] Pek Y. Lum et al. Extracting insights from the shape of complex data using topology. Sci Rep, 3:1236, 2013
[2] Michaël Aupetit. Learning topology with the Generative Gaussian Graph and the EM algorithm. NIPS 2005
[3] M. Maillot, M. Aupetit, G. Govaert. A generative model that learns Betti numbers from a data set. ESANN 2012
[4] P. Gaillard, M. Aupetit, G. Govaert. Learning topology of a labeled data set with the supervised Generative Gaussian Graph. Neurocomputing, 71(7-9): 1283–1299, 2008

Research directions for validation

At step 6), BIC is used to select a « good » simplicial complex based on a statistical criterion on the density $p(x, S, W, \theta)$

- Can we prove it also gives a « good » topological model of the data?
- Or can we find another criterion which does link statistical and topological models properly?
- How the number of data x and the parameters θ of the model impact the « coupling » between density and topology?

From step 4), can a filtration based on the priors π_σ give an interesting topological model?

From steps 2) and 4), can we use multidimensional persistence theory on the number of centers w and the priors π_σ?

Looking for a Post-doc or PhD on these topics, please contact us!