CS 6170: Computational Topology, Spring 2019
Lecture 05
Topological Data Analysis for Data Scientists

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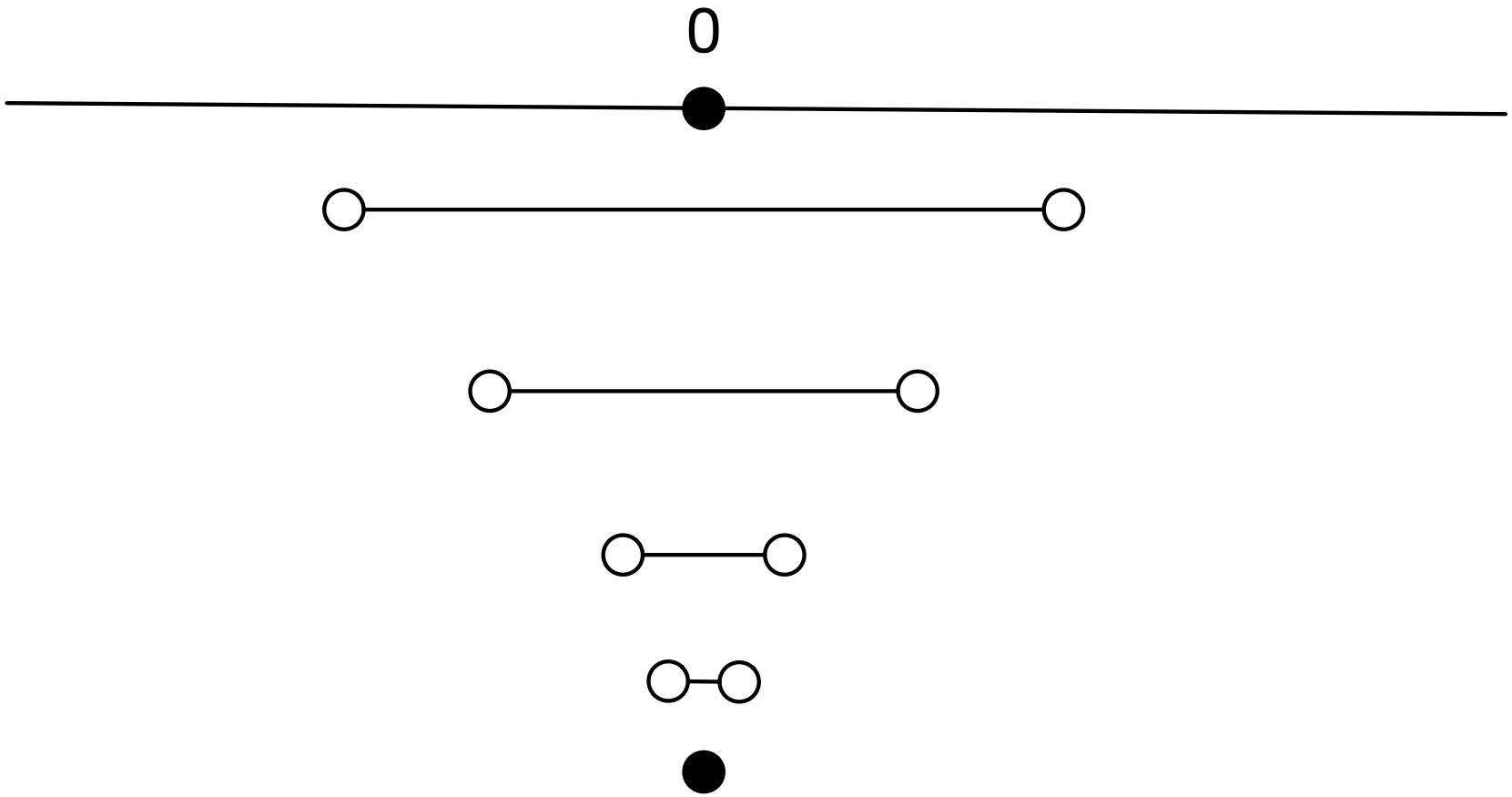
Topology requires a finite number of set intersections?

- Consider the topology on the real line with open intervals
- Imagine a set of intervals $[-\frac{1}{n}, +\frac{1}{n}]$ on the real line, where n goes to ∞.
- Now take the *infinite* number of intersections...
- 0 in the intersection is now a discrete point



Čech complexes and Vietoris-Rips complexes

Book Chapter A.III

Demo:

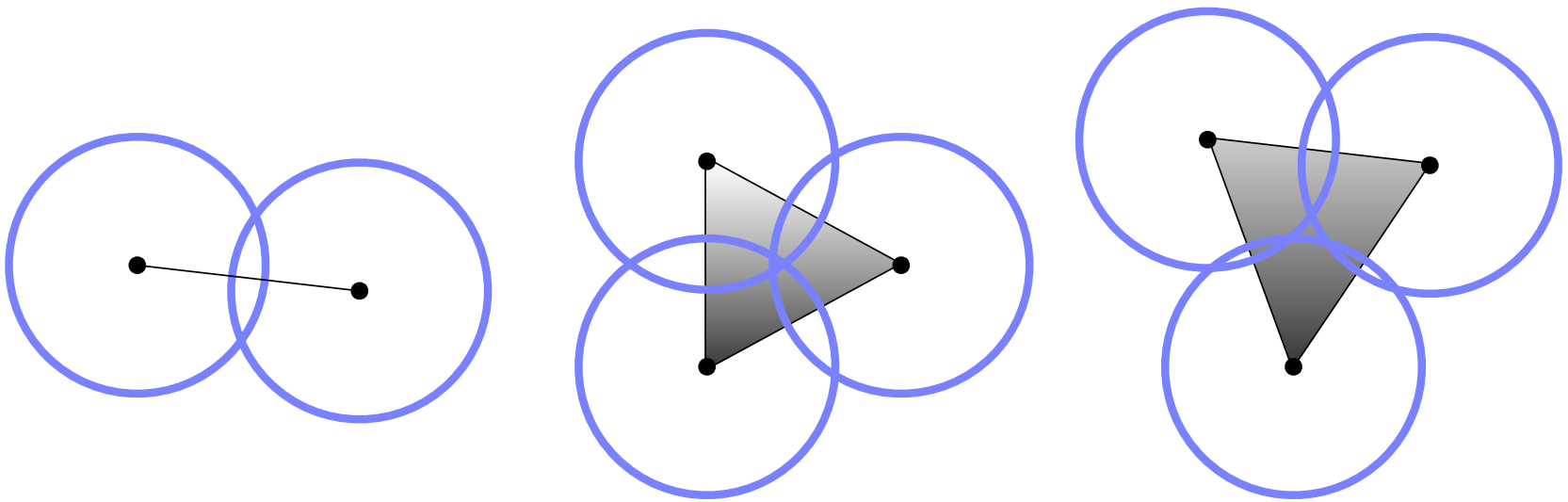
`http://www.sci.utah.edu/~tsodergren/prob_net_vis_working/`

Vietoris-Rips Complex

Given a finite metric space (P, d), e.g., a point cloud $P \subset \mathbb{R}^n$:

Definition

The *Vietoris-Rips complex* of P and r consisting of all subsets of diameter at most $2r$. That is, $\sigma \in \mathcal{R}(r)$ iff $d(p, q) \leq 2r$ for all $p, q \in \sigma$.

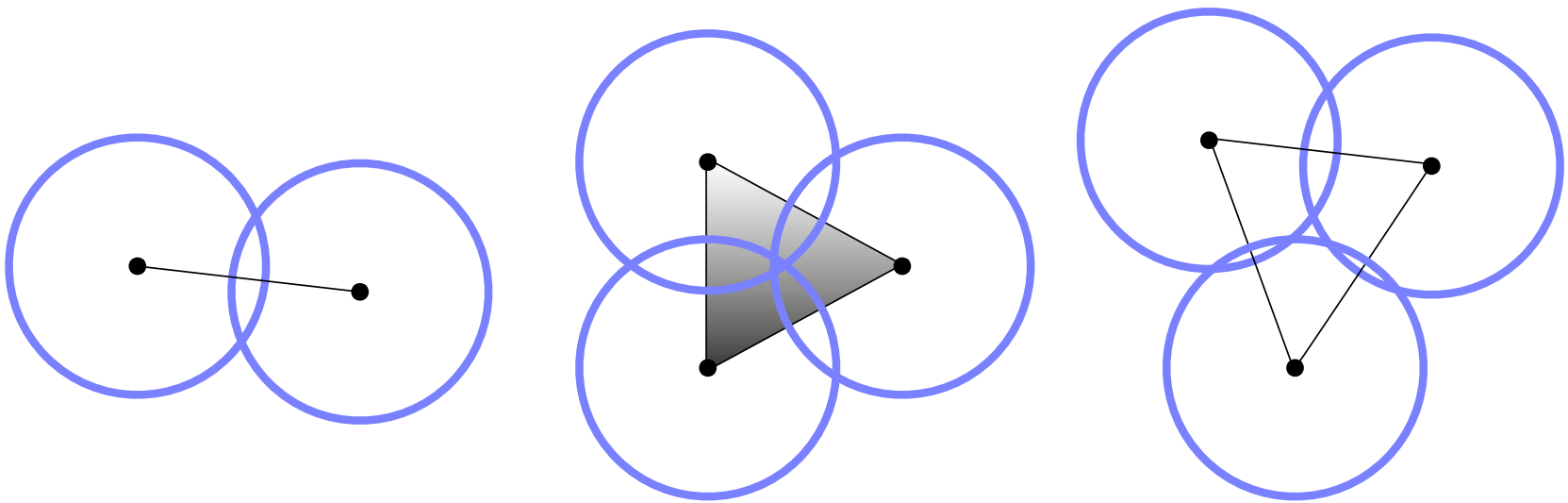


Čech Complex

Given a finite metric space (P, d), e.g., a point cloud $P \subset \mathbb{R}^n$:

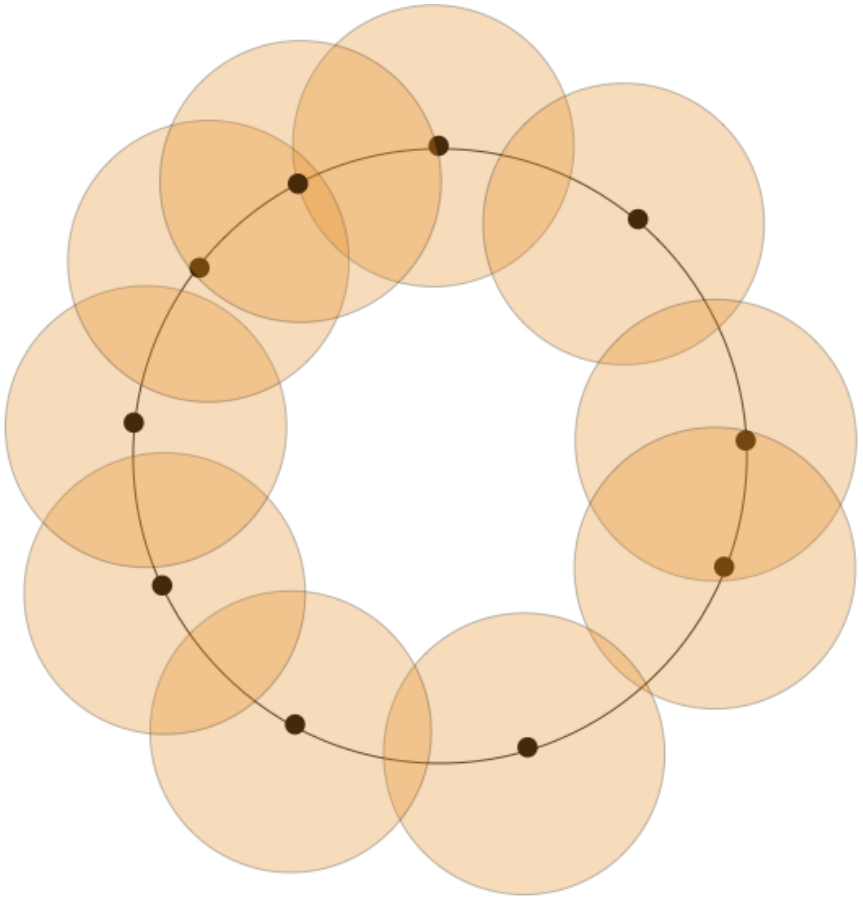
Definition

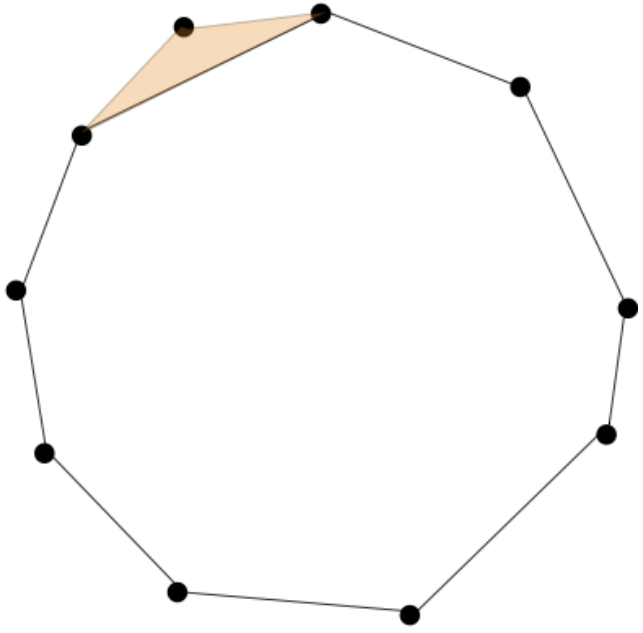
The *Čech complex* of P and r consisting of all subsets whose corresponding sets of r-balls have nonempty intersections. That is, $\sigma \in \mathcal{C}(r)$ iff $\bigcap_{x \in \sigma} B_x(r) \neq 0$.



Sensor Networks

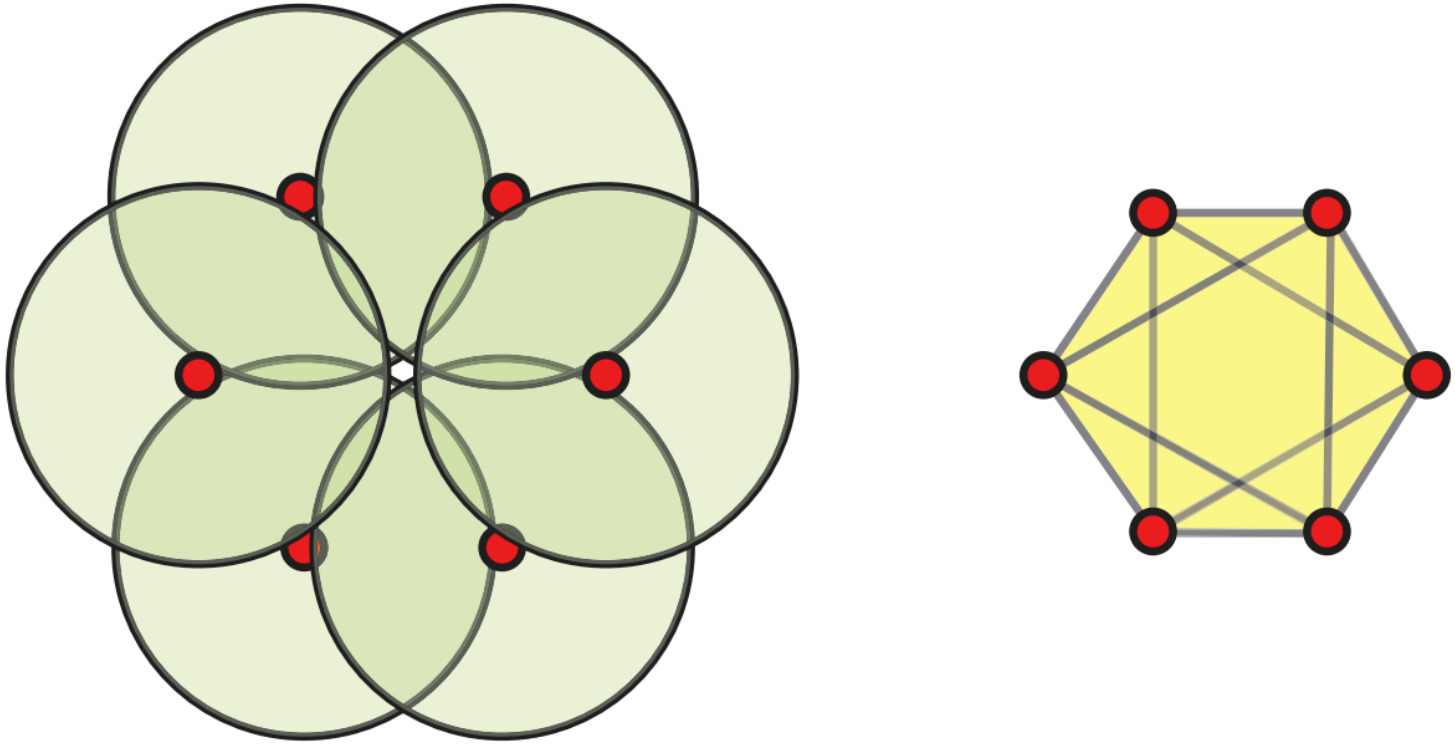
Sensor coverage with Čech complex





https://en.wikipedia.org/wiki/Cech_complex

Rips complex detects "phantom" topological features



Left: Union of balls (Čech). Right: Rips.
Image courtesy of de Silva and Ghrist (2007a).

Using Rips complex to approximate Čech complex

Lemma (Edelsbrunner and Harer (2010), page 62)

Let P be a finite set of points in some Euclidean space and letting $r \geq 0$, then

$$\mathcal{R}(r) \subseteq \mathcal{C}(\sqrt{2}r).$$

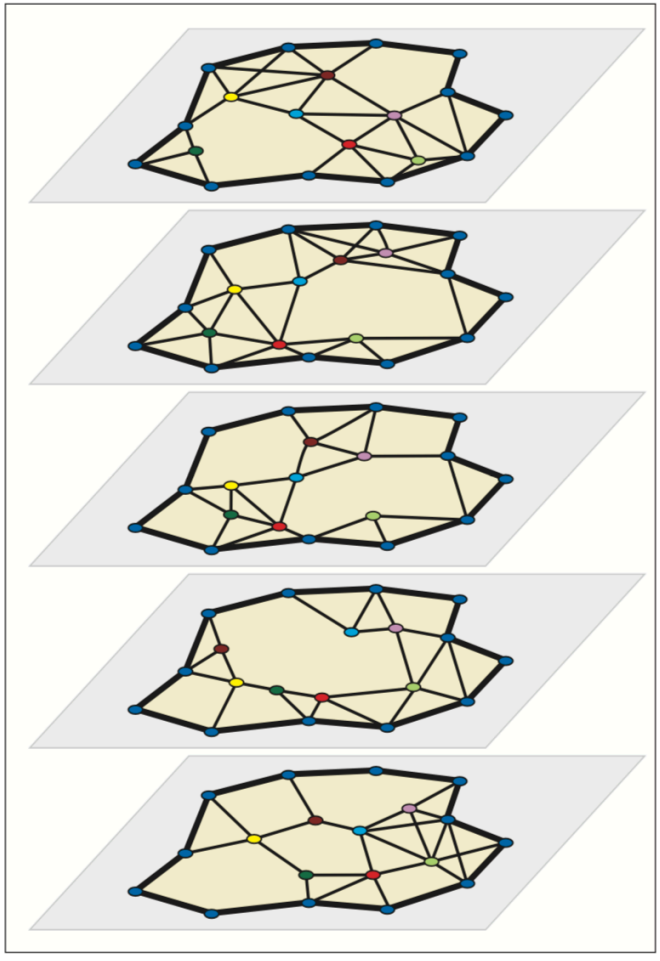
Theorem (de Silva and Ghrist (2007a), Theorem 2.5)

For a point set P in $\mathbb{R}^n$,

$$\mathcal{C}(r) \subset \mathcal{R}(r) \subset \mathcal{C}(\theta r),$$

whenever $\theta \geq \sqrt{\frac{2n}{n+1}}$.

Time-Varying sensor networks



A time-sequence of network graphs for a mobile network. Does this network admit a wandering hole? de Silva and Ghrist (2007b)

Topological Data Analysis for Brain Networks

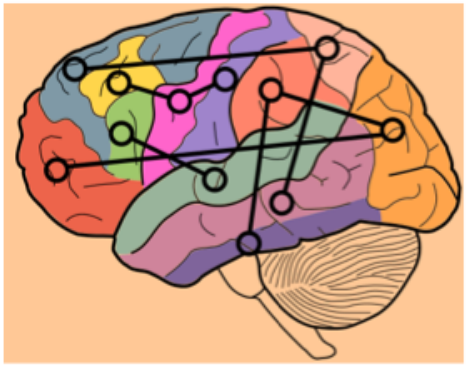
Correlating Brain Network Topology with Autism Severity
Wong et al. (2016)

Big Picture

Goal: Quantify the relationship between brain functional networks and behavioral measures.

Our Contribution: Use topological features based on persistent homology.

Result: Combining correlations with topological features gives better prediction of autism severity than using correlations alone.



functional network

behavior

Motivation

About Autism Spectrum Disorders (ASD):

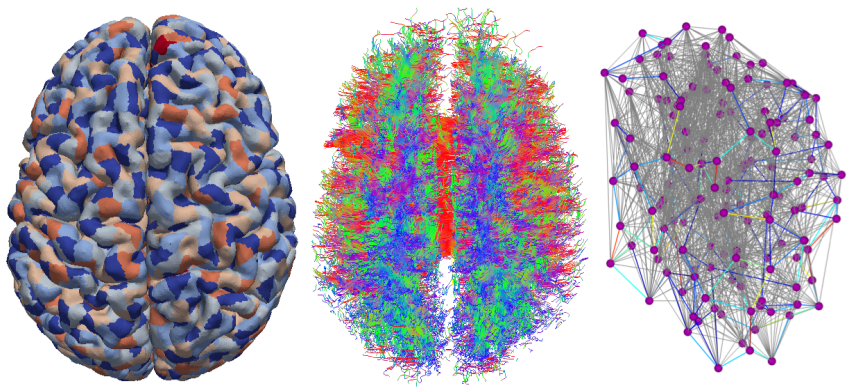
- No cure, causes unknown
- Diagnosis:
  - No systematic method
  - ADOS (Autism Diagnostic Observation Schedule)

Correlate functional brain network to ADOS scores

- Early diagnosis
- Treatment tracking

What is a Brain Network?

- Represents brain regions and pairwise associations
- Computation of Correlation Matrices:
  - Resting state functional MRI (R-fMRI)
  - Preprocessing
  - Define regions of interest (ROIs)
  - Estimate time series signals
  - Compute pairwise associations - Pearson Correlation



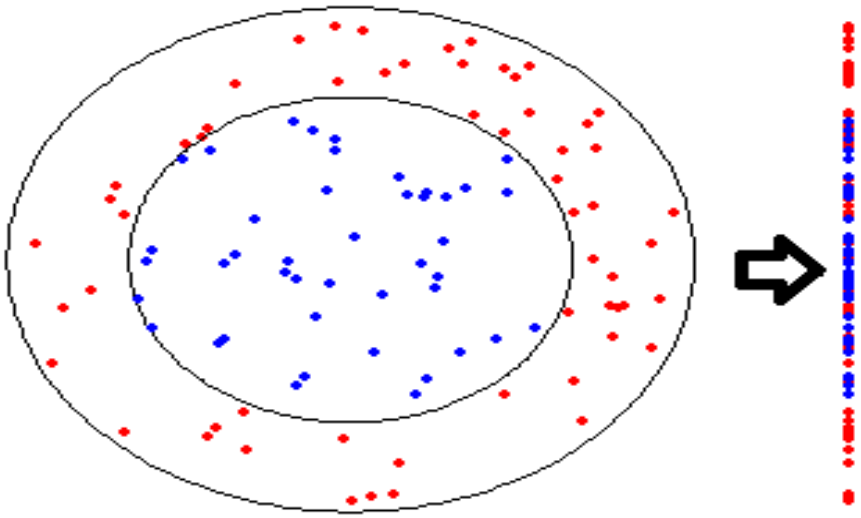
Why Topology?

How to use this data?

- Graph and graph theoretic measures (e.g. small worldness)
  - Require binary associations (thresholding)
- Correlations as features
  - High dimensionality, not enough samples
- Dimensionality reduction: PCA, random projections
  - May lose structures in higher dimensions

Why Topology

Projection - may lose structures in higher dimensions



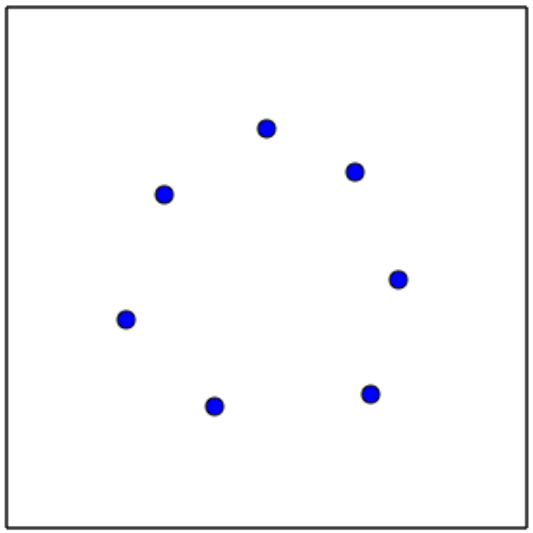
Topology captures structure

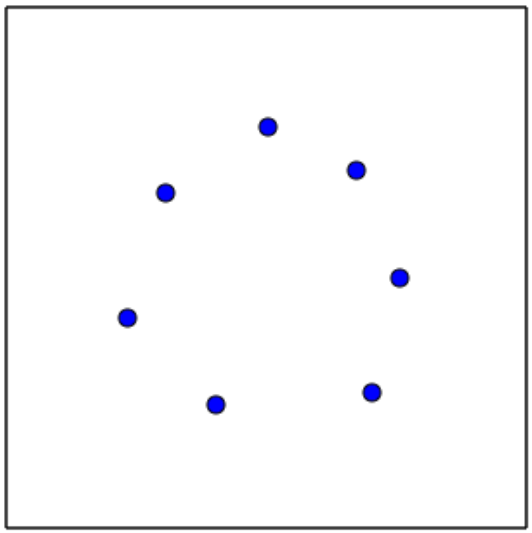
- In higher dimensions
- Across all continuous thresholds

Persistent Homology

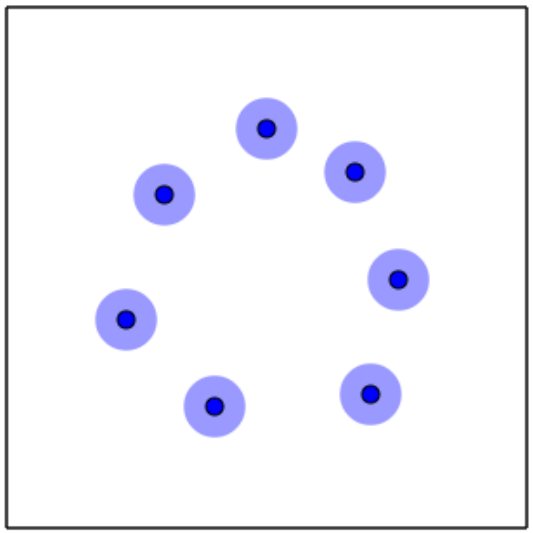
- What are topological features? Homological features:
  - Dim 0 - Connected Components
  - Dim 1 - Tunnels / Loops
  - Dim 2 - Voids
- How to compute them (in a nutshell)?
  - Begin with point cloud
  - Grow balls of diameter t around each point
  - Track features of the union of balls as t increases

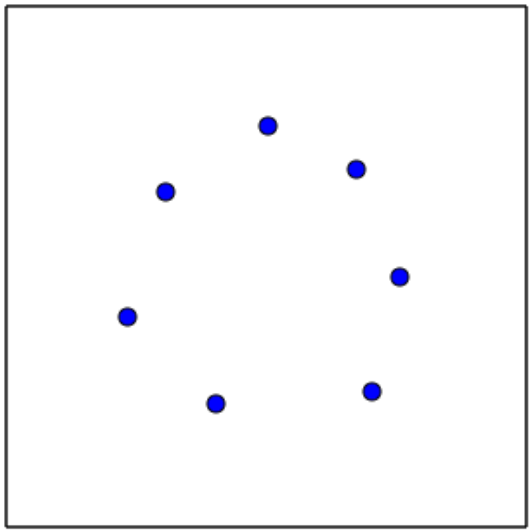
Persistent Homology



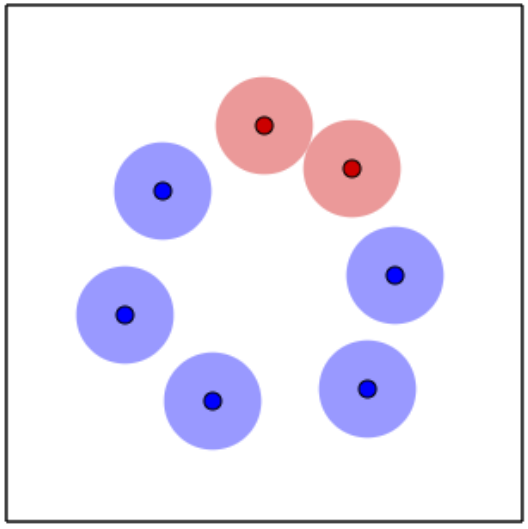


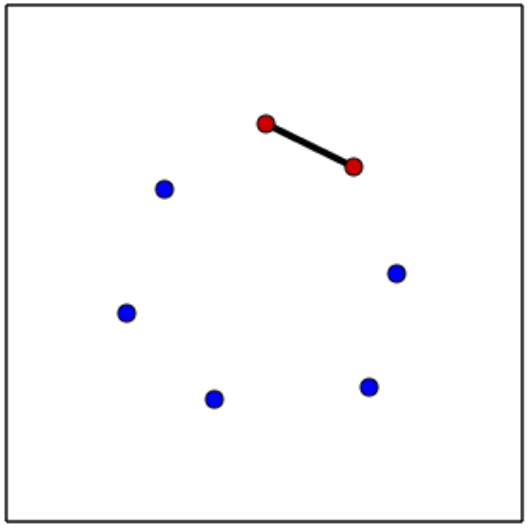
Persistent Homology



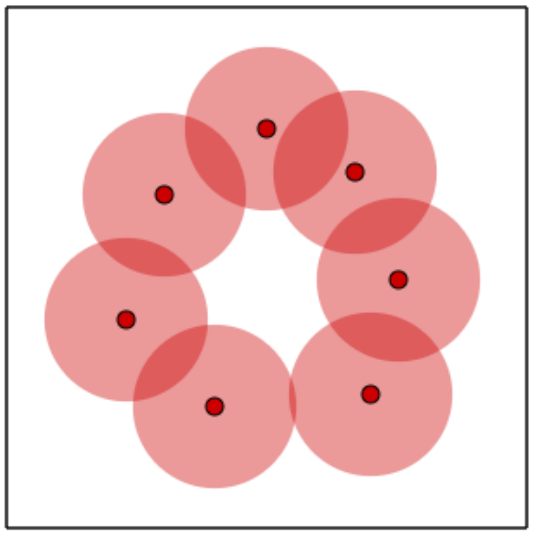


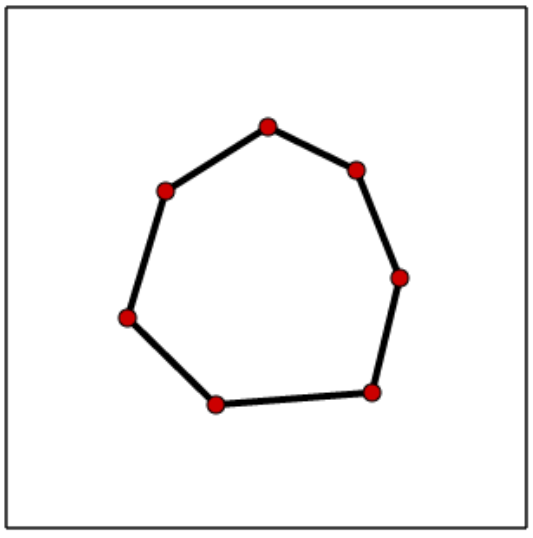
Persistent Homology



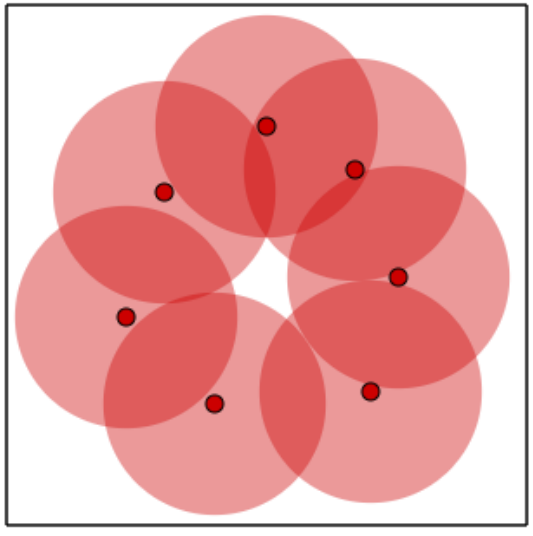


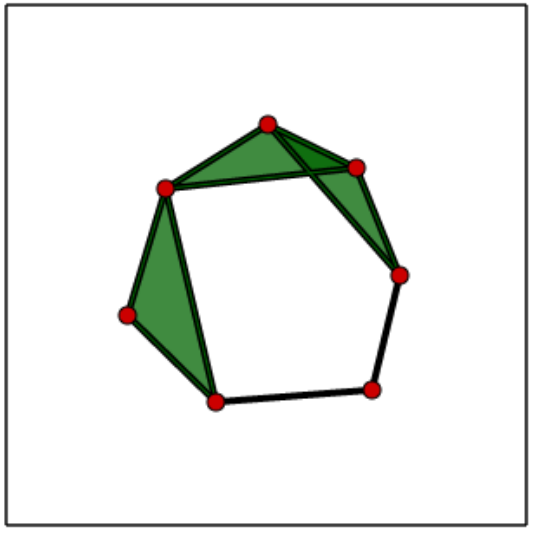
Persistent Homology



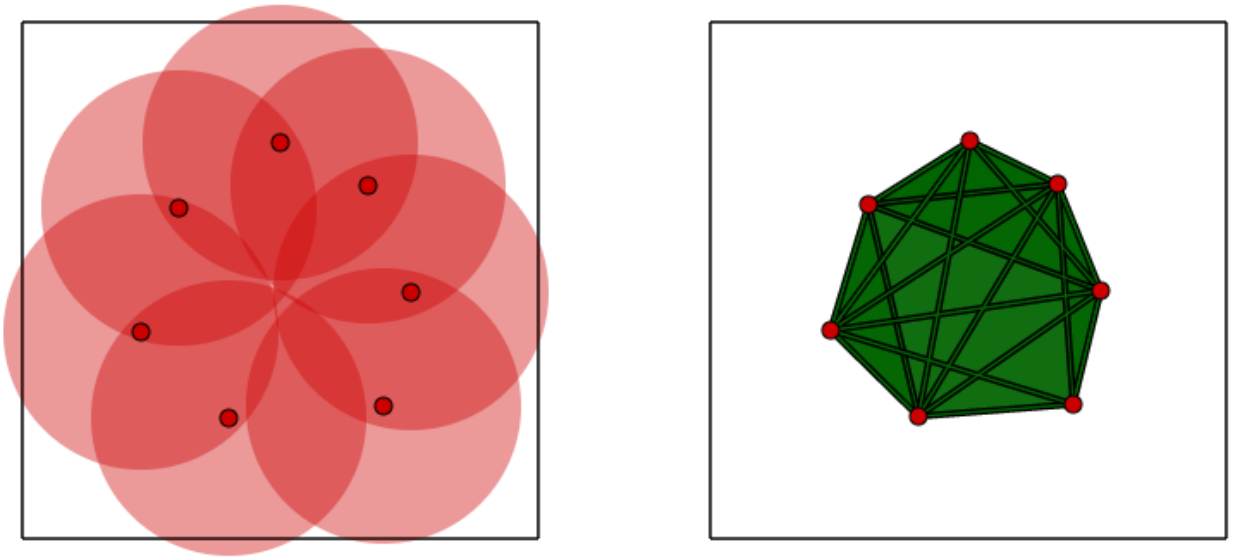


Persistent Homology





Persistent Homology



Persistence Diagrams

Persistent homological features - encoded as barcodes or persistent diagrams

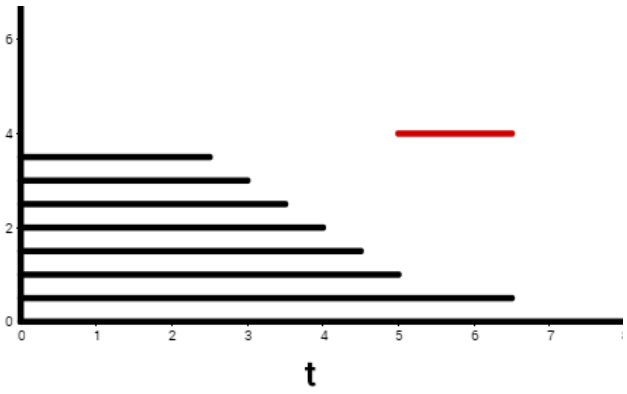


Figure: Barcode

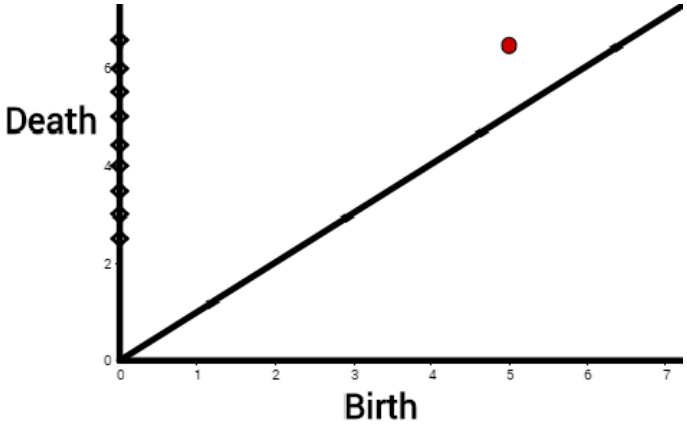
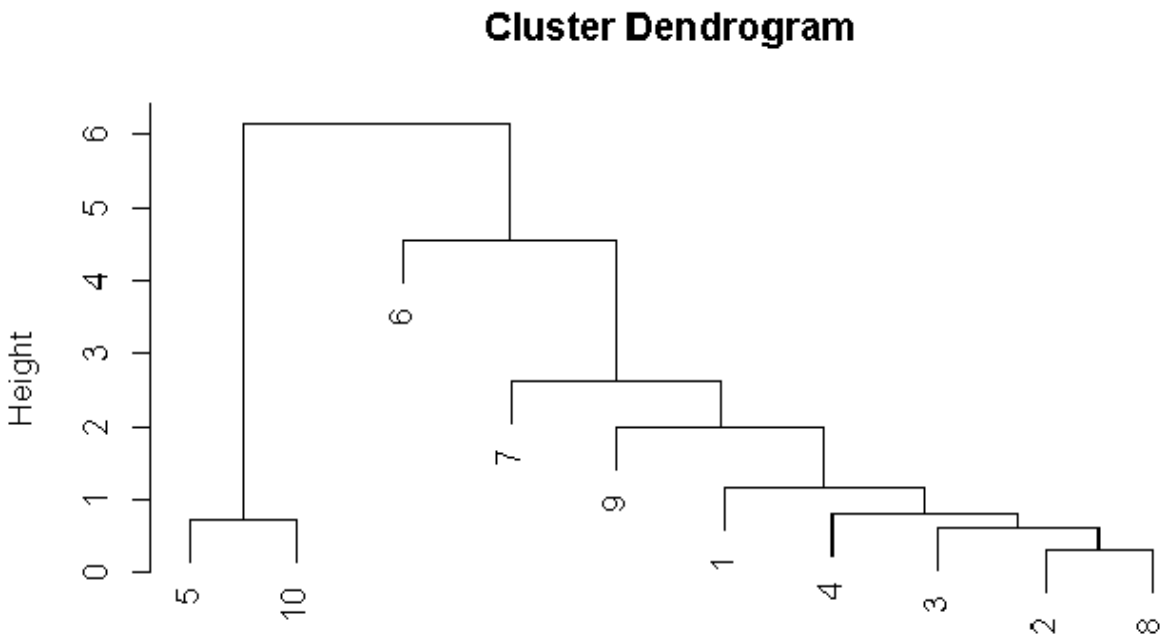


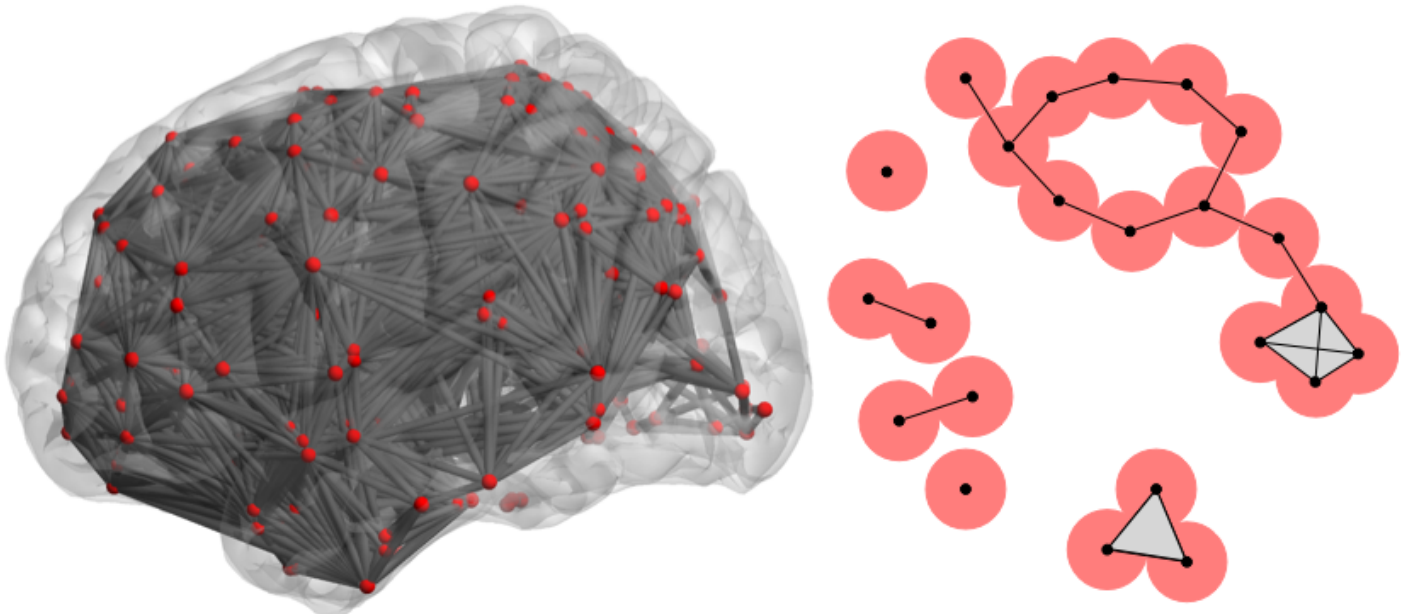
Figure: Persistence Diagram

Interpretation of Connected Components

- Dim 0 features - hierarchical clustering



Computing Topological Features for Brain Networks



Partial Least Squares (PLS) Regression

A dimensionality reduction technique that finds two sets of latent dimensions from datasets X and Y such that their **projections** on the latent dimensions are **maximally co-varying**.

- X - features from brain imaging: correlations, topological features (zero mean)
- Y - clinical measure of behavior: ADOS scores (zero mean)

PLS models the relations between X and Y by means of **score vectors**.

PLS Regression

- n - number of data points
- X - predictor/regressor $(n \times N)$, Y - response $(n \times M)$
- PLS - decompose X, Y such that:

$$X = TP^T + E$$
$$Y = UQ^T + F$$

Where

- T, U - latent variables/score vectors $(n \times p)$, factor matrices
- P $(N \times p)$, Q $(M \times p)$ - orthogonal loading matrices
- E $(n \times N)$, F $(n \times M)$ - residuals/errors

- T, U are chosen such that projections of X, Y, that is, T and U, are maximally co-varying.

PLS Regression: the Algorithm

Iterative NIPALS algorithm Wold (1975) (nonlinear iterative partial least squares)

- Find first latent dimension

  i.e. find vectors w, c such that

  $$t = Xw, \quad u = Yc$$

  have maximal covariance
- Deflate previous latent dimensions from X, Y and repeat

Kernel PLS

Kernel form of NIPALS algorithm (kPLS)

1. Initialize random vector u
2. Repeat until convergence
   a. $t = Ku/\|Ku\|$
   b. $c = Y^T t$
   c. $u = Yc/\|Yc\|$
3. Deflate $K = (I - tt^T)K(I - tt^T)$
4. Repeat to compute subsequent latent dimensions

Data

- 87 Subjects: 30 Control, 57 ASD
- ADOS scores: 0 to 21
- 264 ROIs (Power regions)
- 264×264 correlation matrix.
- 34,716 distinct pairwise correlations per subject.

Experiments

- Given: Correlation matrices
- Map to metric space

$$d(x, y) = \sqrt{1 - \mathsf{Cor}(x, y)}$$

- Compute persistence diagrams
- Define inner product of persistence diagrams Reininghaus et al. (2015) (i.e. kernel): Given two persistence diagrams F, G

$$k_\sigma(F, G) = \frac{1}{8\pi\sigma} \sum_{p \in F} \sum_{q \in G} e^{-\frac{\|p-q\|^2}{8\sigma}} - e^{-\frac{\|p-\bar{q}\|^2}{8\sigma}}$$

where for every $q = (x, y) \in G$, $\bar{q} = (y, x)$

Experiments

Performed experiments with 3 kernels:

1. K^{Cor} - Euclidean dot product of vectorized correlations
2. $K^{TDA} = w_0 K^{TDA_0} + (1 - w_0) K^{TDA_1}$
   - K^{TDA_0} - using only Dim 0 features
   - K^{TDA_1} - using only Dim 1 features
3. $K^{TDA+Cor} = w_0 K^{TDA_0} + w_1 K^{TDA_1} + (1 - w_0 - w_1) K^{Cor}$

Baseline predictor - mean ADOS score

Experiments

- Leave one out cross validation over parameters
  - σ_0, σ_1 - $(\log_{10} \sigma)$ from -8.0 to 6.0 by 0.2
  - w_0, w_1 - from 0.0 to 1.0 by 0.05
- k^{TDA} parameters: $\sigma_0 = -6.6$, $\sigma_1 = 1.8$, $w_1 = 0.95$
- $k^{TDA+Cor}$ parameters: $\sigma_0 = -7.8$, $\sigma_1 = 2.8$, $w_0 = 0.1$, $w_1 = 0.4$
- Compute RMSE
- Permutation test for significance

Results and Conclusions

	RMSE	ADOS mean	K^{TDA}	K^{cor}
ADOS mean	6.4302	-	-	-
K^{TDA}	6.3553	0.316	-	-
K^{cor}	6.0371	0.055	0.095	-
$K^{\mathrm{TDA+cor}}$	**6.0156**	**0.048**	0.075	0.288

Table: ADOS prediction results. Columns 2 to 4 are p-values for the permutation test of improvement of row method over column method.

Result Highlights:

- Baseline RMSE: 6.4302
- $K^{TDA+Cor}$:
  - Only method statistically significant over baseline
  - Permutation test p-value: 0.048
  - RMSE: 6.0156

Conclusion

- Augmenting correlations with topological features gives a **better** prediction of autism severity than using correlations alone
- (Hopefully) topological features derived from R-fMRI have the **potential** to explain the connection between functional brain networks and autism severity

Future Work

- Alternatives to correlation
- Different distance metric
- Different kernel
- Multi-site data
- Classification (combine with TDA features)

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