Kernel Partial Least Squares Regression for Relating Functional Brain Network Topology to Clinical Measures of Behavior

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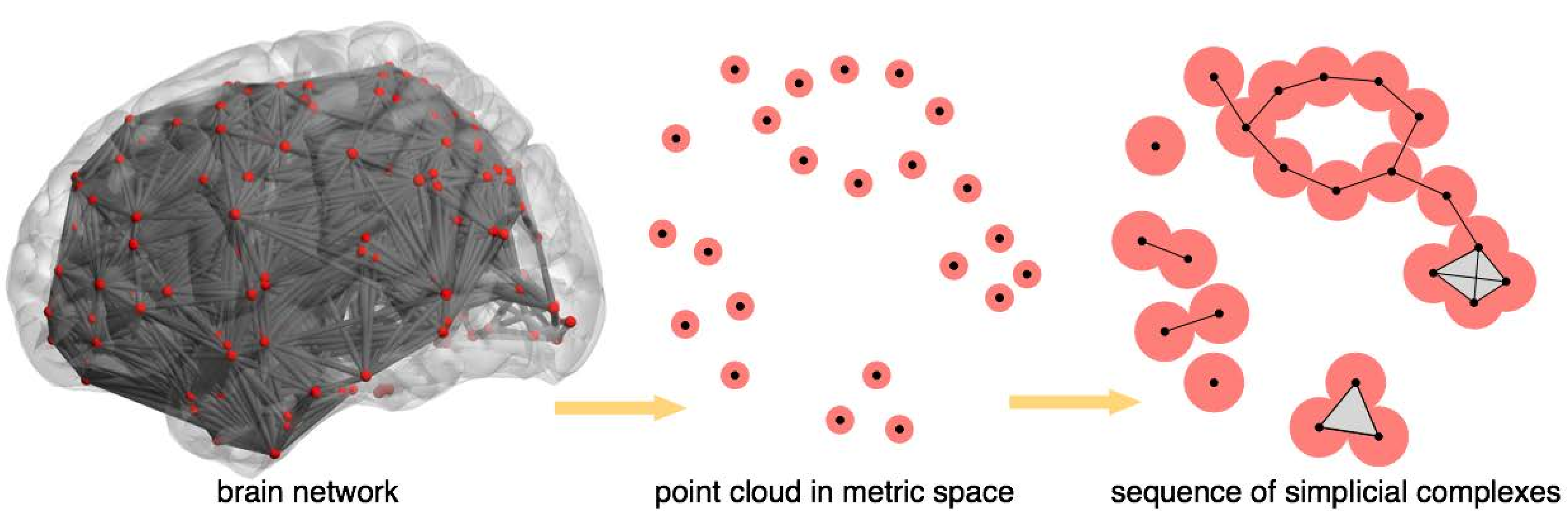
Overview

We propose a method for analyzing relationships between functional brain networks and behavioral phenotypes.

We map **topological data features** extracted from resting-state fMRI networks to a kernel space and use **kernel partial least squares** (kPLS) regression to quantify their relationship to autism. The advantages are:

- Typical correlation-based methods use thresholds to determine the existence of an edge in the network. Topological features capture network organization across all threshold values.
- Multiple image features can be easily combined by a summation of kernels.

Topology of Brain Networks

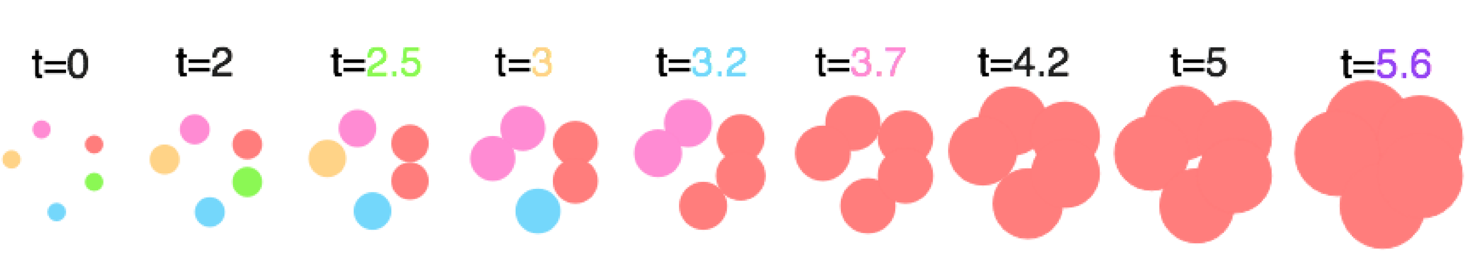


Procedure:

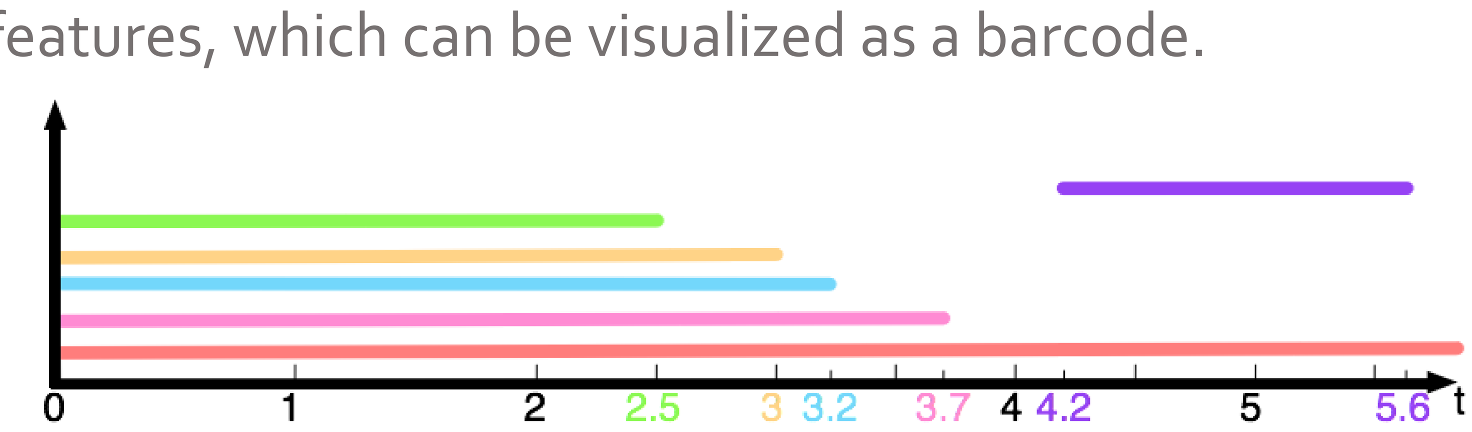
- For each subject, map the nodes from a brain network to points in a metric space using the distance measure,

$$d(u,v) = \sqrt{(1 - corr(u,v))}.$$

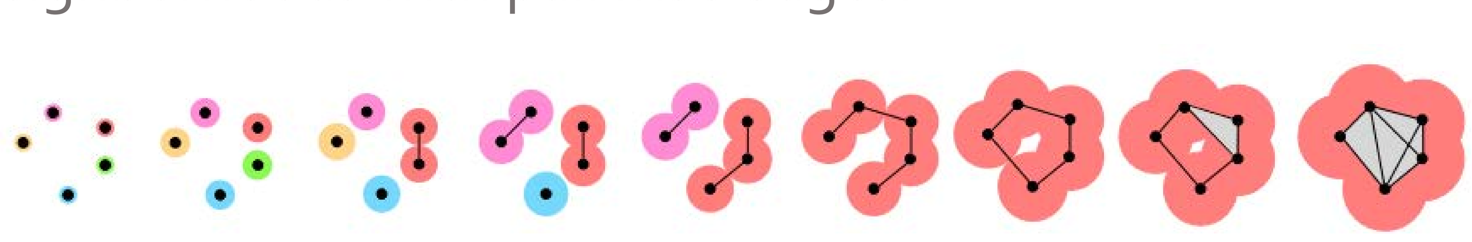
- Grow the radius of a neighborhood around each point. Neighborhoods begin to merge.
- Track the 0-,1-,2-dim topological features (connected components, holes, and voids) that appear and disappear over time.



Persistent homology follows the birth and death times of these features, which can be visualized as a barcode.



It is equivalent to capturing the topological changes of the *Rips complexes*, formed by connecting the points in intersecting neighborhoods with pairwise edges.



References

[1] Rosipal, Roman, and Leonard J. Trejo. "Kernel partial least squares regression in reproducing kernel hilbert space." *The Journal of Machine Learning Research* 2 (2002): 97-123.

[2] Reininghaus, Jan, et al. "A stable multi-scale kernel for topological machine learning." *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*. 2015.

Kernel Partial Least Squares

PLS projects two datasets, X and Y, of sizes $n \times N$ and $n \times M$ down to p latent dimensions that maximally covary. kPLS [1] extends this, assuming that X is mapped by Φ to a higher dimensional inner product space $\mathcal{F}$.

kPLS Algorithm

$$t = \Phi(x)\Phi(x)^T u = Ku$$
$$\|t\| \to 1$$
$$c = Y^T t$$
$$u = Yc$$
$$\|u\| \to 1$$

K : Gram matrix of X

$K(x,x') : \langle \Phi(x), \Phi(x') \rangle_{\mathcal{F}}$

t, u : covarying latent variables

c : loadings for Y

Once all the latent dimensions are found, the regression from kernel to Y is $\hat{Y} = \Phi(x)B = KU(T^T KU)^{-1} T^T Y.$

TDA Kernel

We take all subject persistence barcodes to construct a multi-scale topological kernel [2] with stability properties,

$$K_\sigma^{TDA}(A,B) = \frac{1}{8\pi\sigma} \sum_{p \in A, q \in B} e^{-\frac{||p-q||^2}{8\sigma}} - e^{-\frac{||p-\bar{q}||^2}{8\sigma}}$$

where for every $q = (a,b) \in B,\ \bar{q} := (b,a).$

Experiments

Goal Predict ADOS score from resting state fMRI using data from one site in the ABIDE dataset (30 control, 57 ASD subjects)

Results Compared with using just raw correlations from 264 ROIs (d=34716), augmentation with topological features improves predictive power.

We did LOOCV and evaluated the RMSE of the predictions. We used the following comparisons:

- K^{cor}: Linear kernel from correlation matrices by taking Euclidean dot products between subjects
- K^{TDA_0} and K^{TDA_1}: 0-,1-dim TDA feature kernels
- $K^{\text{TDA+cor}} = w_0 K^{\text{TDA}_0} + w_1 K^{\text{TDA}_1} + (1 - w_0 - w_1) K^{\text{cor}}$: the combined kernel with 4 parameters to cross validate over. Weights w_0, w_1 in the range 0 to 1 by 0.05, and log kernel sizes $\log_{10}(\sigma_0), \log_{10}(\sigma_1)$ from -8 to 6 by 0.2
- ADOS mean baseline: mean from n-1 subjects to predict leave-out subject. We also looked at random noise which performed worse than this baseline.

	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	-
$K^{\text{TDA+cor}}$	**6.0156**	**0.048**	0.075	0.288

We used permutation tests to get a p-value for the significance of the results.

Acknowledgements

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