Principal component analysis in treespace

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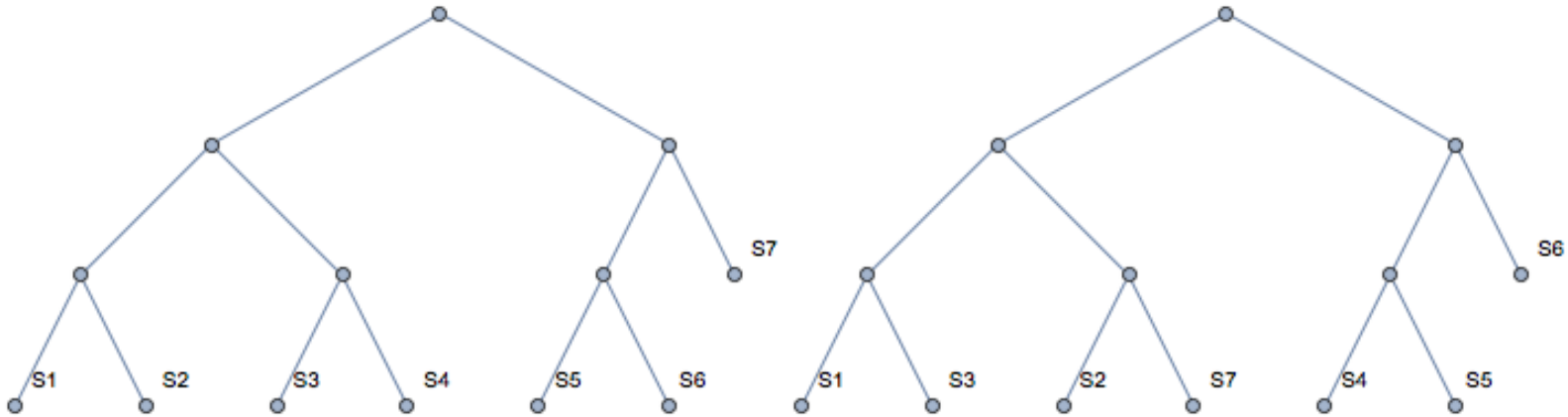
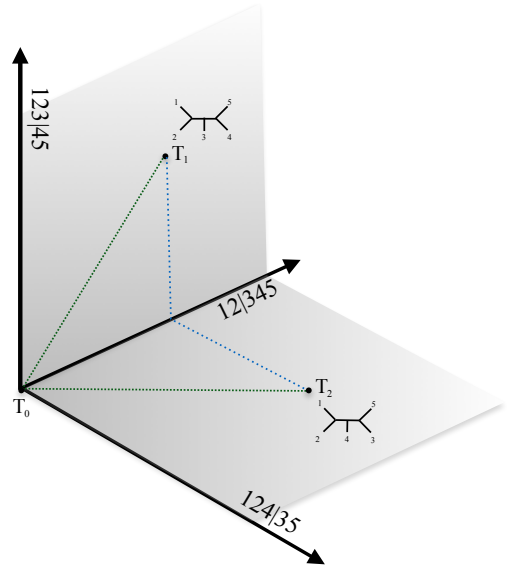
Distances between phylogenetic trees

- Given two trees (rooted or unrooted) on the same set of leaves (taxa), to what extent to they differ?



- Metrics on trees: Nearest Neighbor Interchange (NNI), Robinson-Foulds (RF) Δ, Subtree-Prune-Regraft (SPR), Tree Bisection and Reconnection (TBR), Billera-Holmes-Vogtmann (BHV), ...

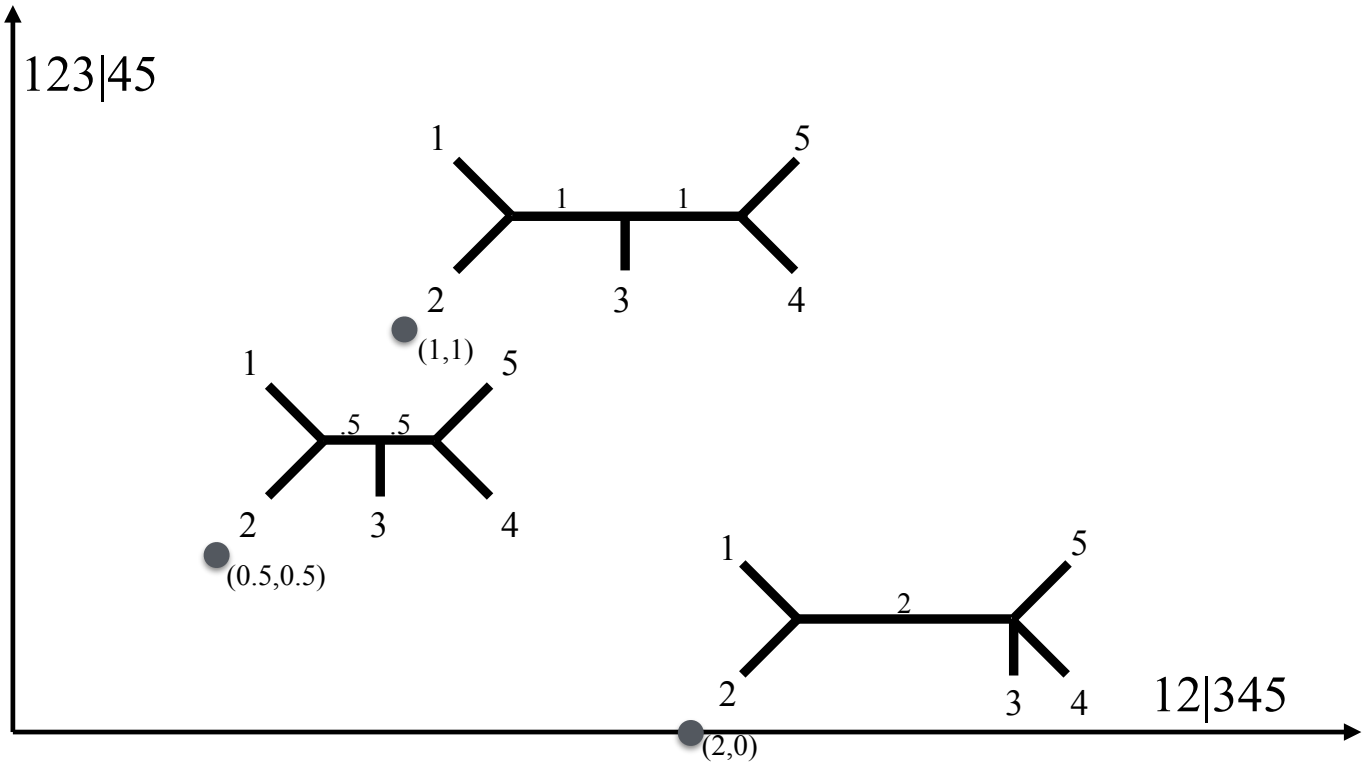
Trees as Vectors



	1 | 2345	2 | 1345	3 | 1245	4 | 1235	5 | 1234	12 | 345	13 | 245	14 | 235	15 | 234	23 | 145	24 | 135	25 | 134	34 | 125	35 | 124	45 | 123
$T_0 = (1,2,3,4,5)$	1	1	1	1	1	0	0	0	0	0	0	0	0	0	0
$T_1 = ((1,2),(3,(4,5))$	1	1	1	1	1	1	0	0	0	0	0	0	0	0	1
$T_2 = ((1,2),(4,(3,5))$	1	1	1	1	1	1	0	0	0	0	0	0	0	1	0

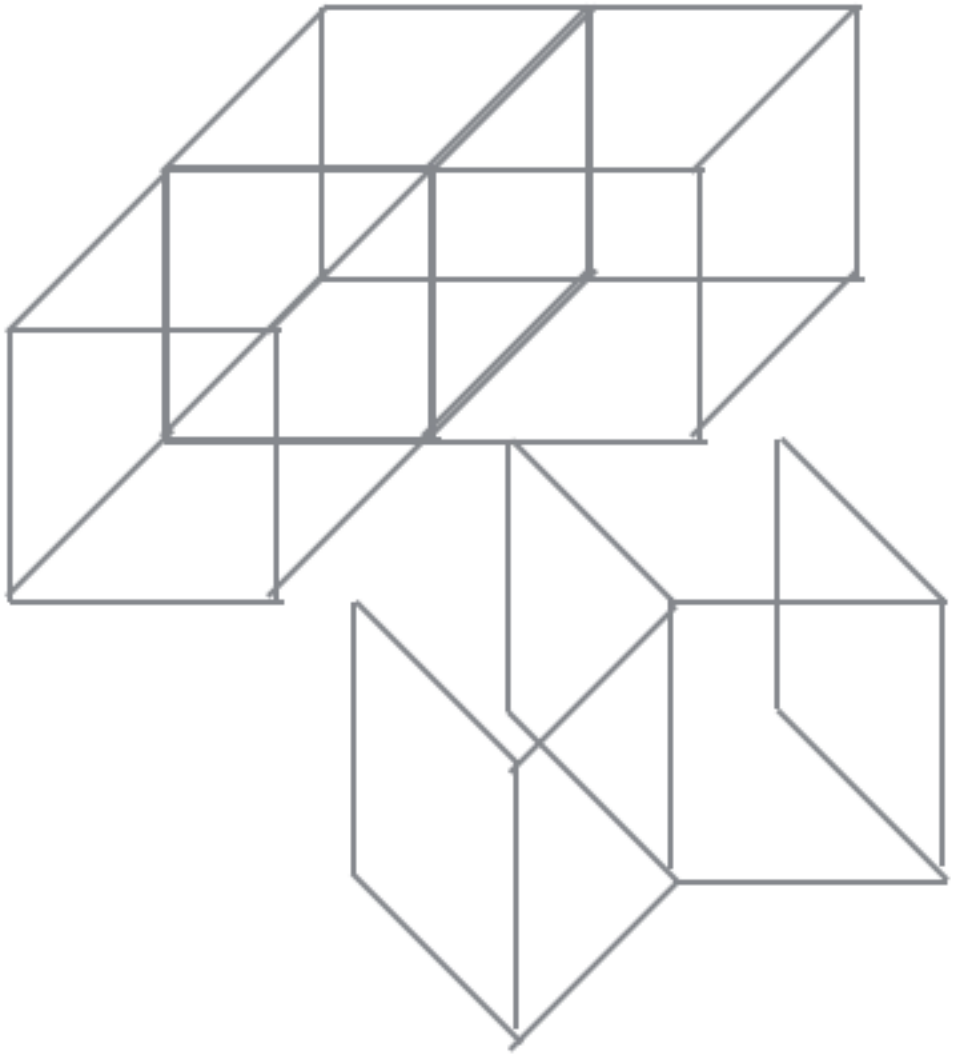
Billeara-Holmes-Vogtmann space

- Trees on fixed n taxa, edge lengths positive reals
- Edges to leaves have fixed length 1
- Form a space with a metric which is locally Euclidean



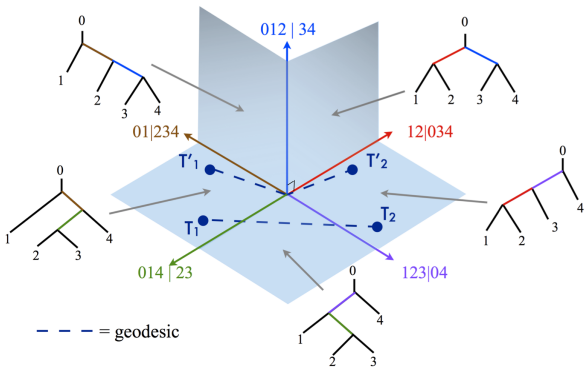
Billera-Holmes-Vogtmann treespace

- Adjacency of orthants: two orthants of dimension k share a face of dimension l if they have l edges in common.
- Gives gluing of orthants to obtain space



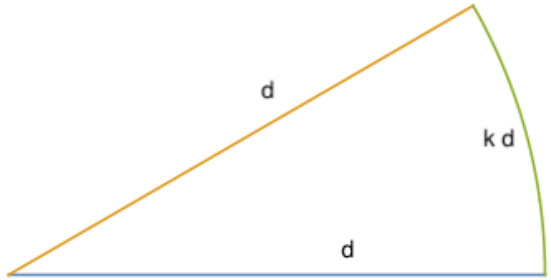
Finding geodesics in treespace

- Piecewise Euclidean segments in a sequence of orthants
- Many cells to consider
- First algorithms exponential
- Polynomial-time algorithm of order $O(n^4)$ of Owen-Provan (2011) uses incompatibility graph of edges to compute which edges to drop and introduce successively.
- Owen-Provan algorithm foundational for computing means, interpolations, variances, principal components, ...

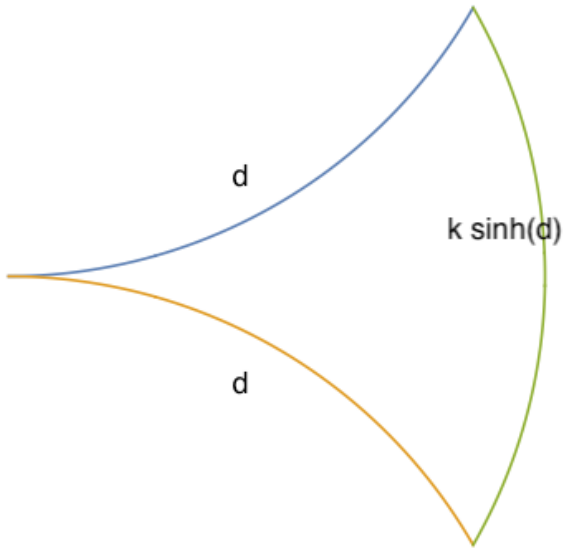


Divergence of geodesics in hyperbolic space

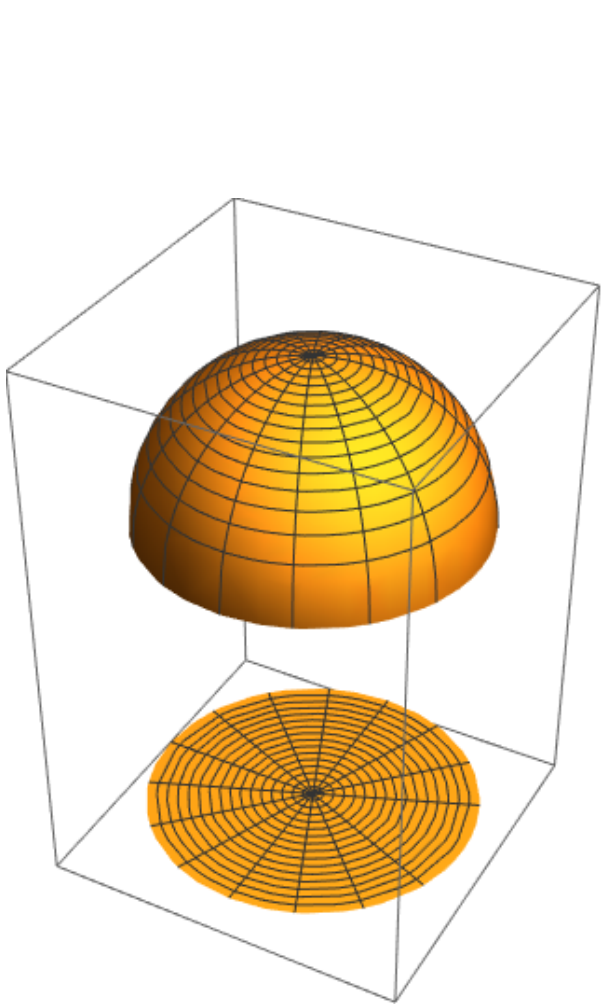
Euclidean: lengths of paths between points on two geodesic rays from X at angle θ at distance d increases linearly in d:

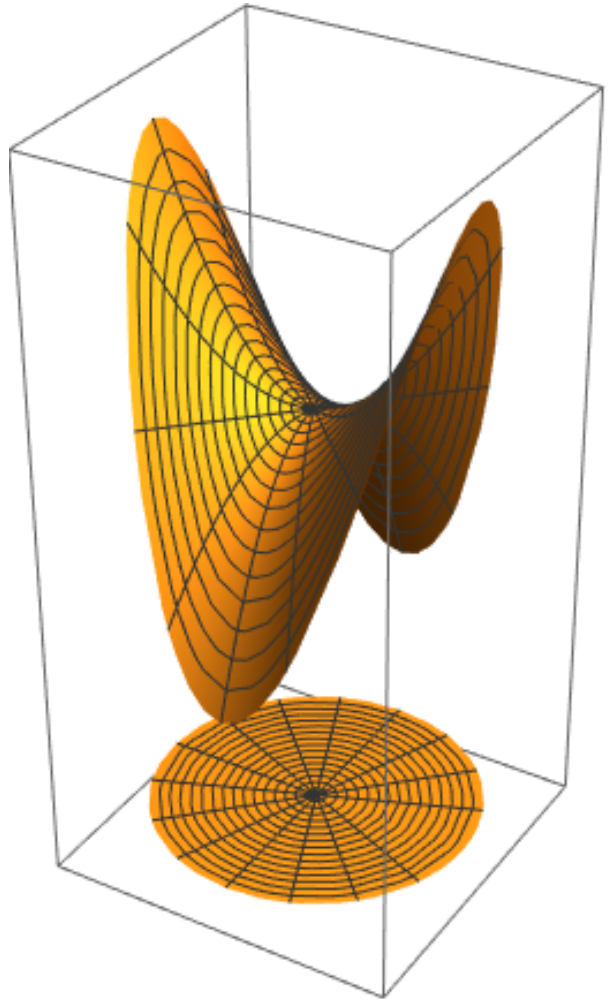


Hyperbolic: lengths of paths between points on two geodesic rays from X at angle θ at distance d outside the ball increases exponentially



Projections from non-positive to Euclidean have distortion





Capturing sets of trees via dimensionality reduction

Hillis, Heath, St. John (2005)
Given a set of trees T_i:

- Can construct pair-wise distance matrix wrt. preferred metric
- Embed this approximately in high-dimensional Euclidean space
- Take traditional Euclidean MDS to project to lower-dimensional space that best captures variances

Advantages: uses effective tools, gives valuable visualizations
Disadvantages: assumes a Euclidean structure

Finding geodesics capturing the first principal component

Given a set of trees $\{T_i\}$:

- Nye (2011, 2014): efficient algorithm to find endpoints of a geodesic γ where projections via BHV onto γ are maximally correlated with pairwise BHV distances
- Feragen, Owen (2013, 2015): generalized Nye's algorithm for medical imaging of airway trees in healthy and diseased lungs
- Cleary, Feragen, Owen, Vargas (2015, 2020): iterate projections onto geodesics
- Nye et. al (2017): projections onto 2-dimensional subsurfaces of BHV space.

Iterated projections

Given a set of trees $\{T_i\}$:

- Find γ the geodesic best capturing the projected distances, parameterize via $[0, 1]$.
- For each T_i, find point on γ closest, to give coordinates t_i
- Bin the trees into subsets S_j by coordinates t_i
- Repeat the analysis on the smaller subsets S_j

Lives a collection of piecewise projections
Can iterate to get subsets $S_{j,k,\ldots}$

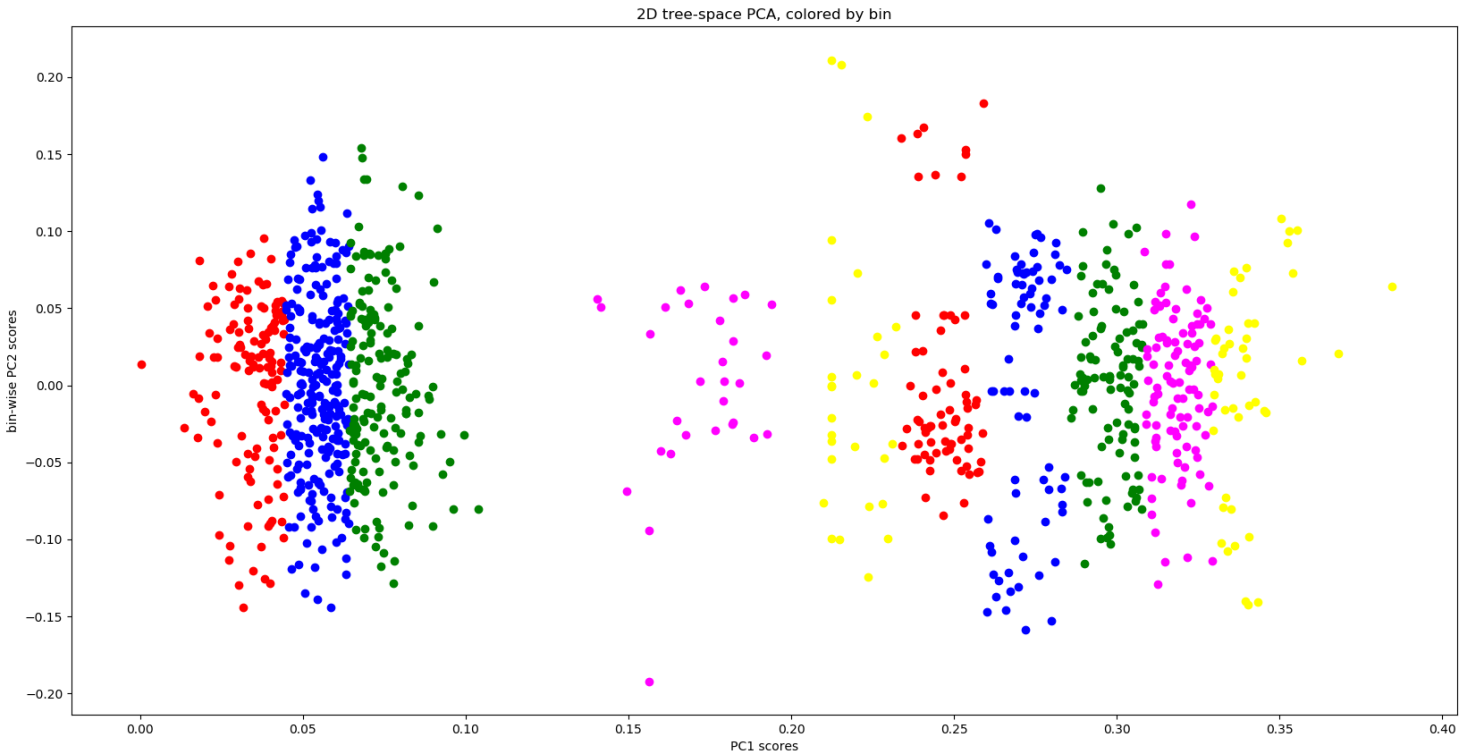
Two dimensional case

Given a set of trees $\{T_i\}$:

- Find γ, backbone of the entire collection
- Bin trees into say 10 subsets along projections onto γ
- Find γ_0 to γ_9, geodesics for those 10 subsets
- Give coordinates (x, y) to trees based upon their projections onto γ and the relevant γ_i
- Use these coordinates to plot and visualize data

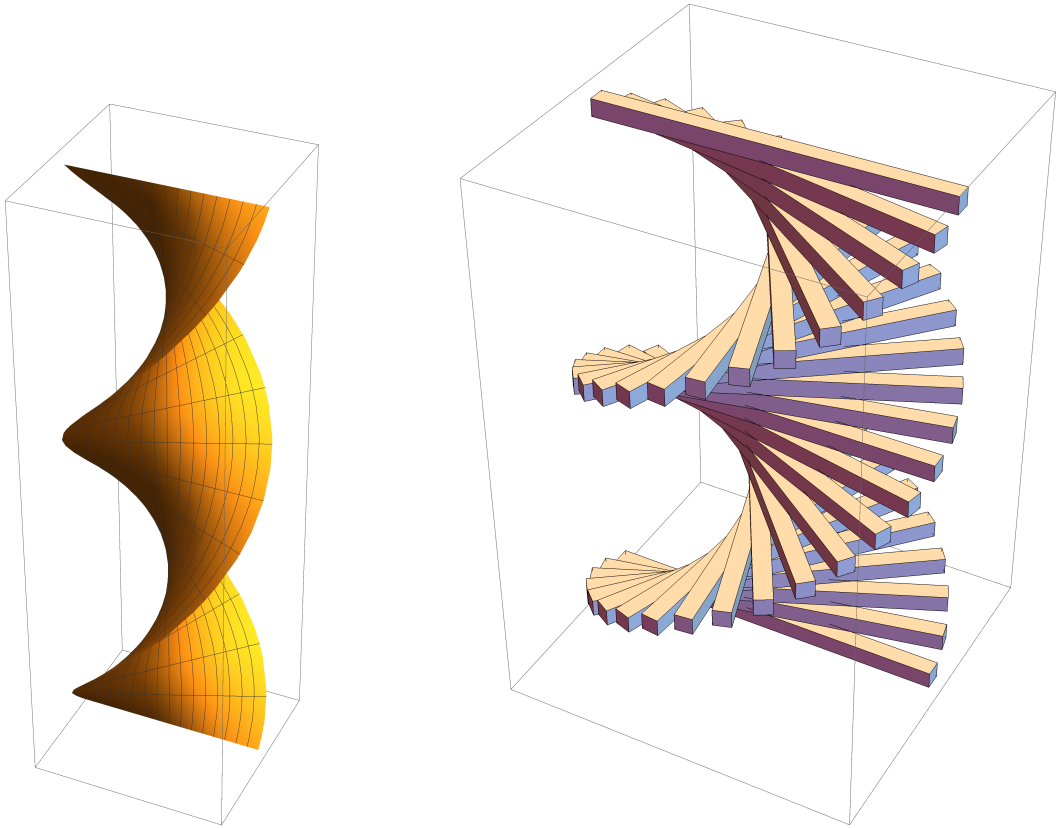
Example

VL3 dataset: 442 trees on 50 taxa, GARTFase Beiko et al. (2006), alignments bacterial and archaeal sequences of protein-coding genes



Piecewise approximation

Approximate helicoid via backbone and perpendicular parts of changing direction:

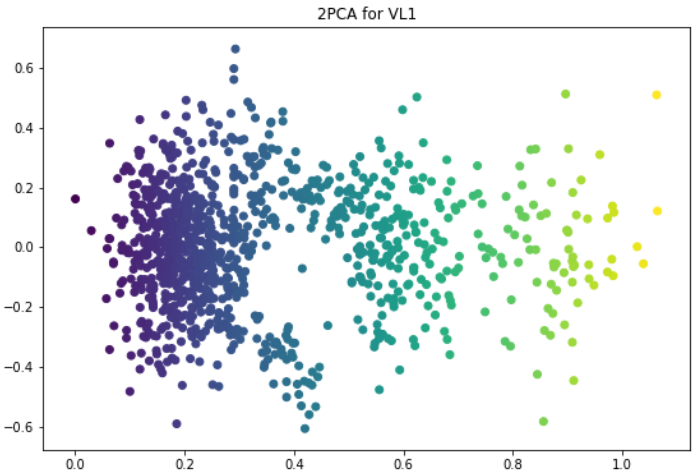


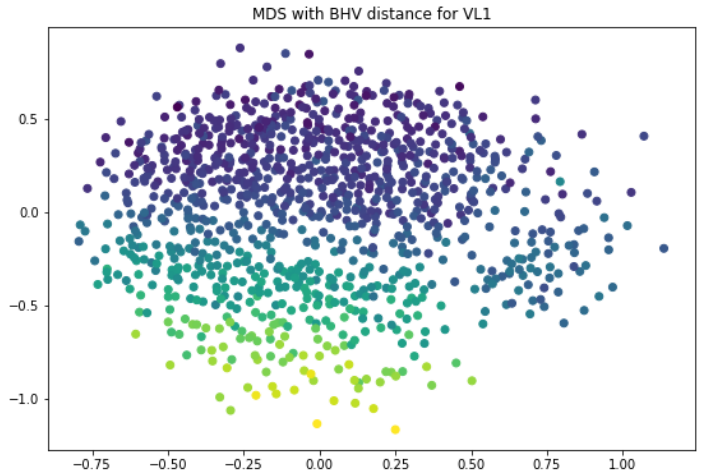
Properties

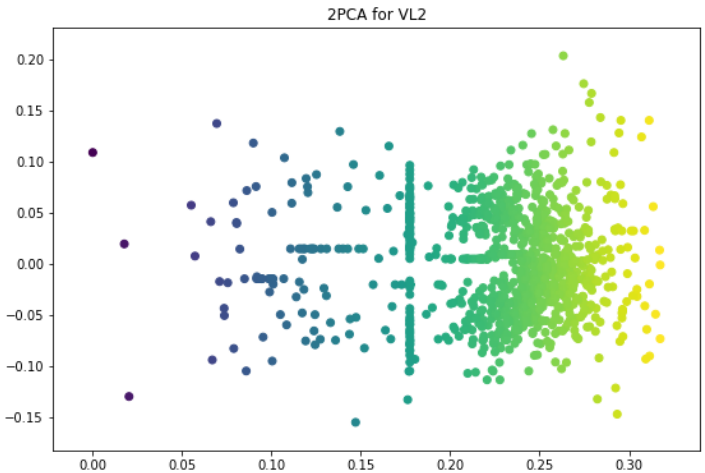
- Projections are optimized locally on subsets, more robustness with respect to far off points
- Choices about orientation made to maximize correlation
- Uses: cluster identification, visualizing distribution

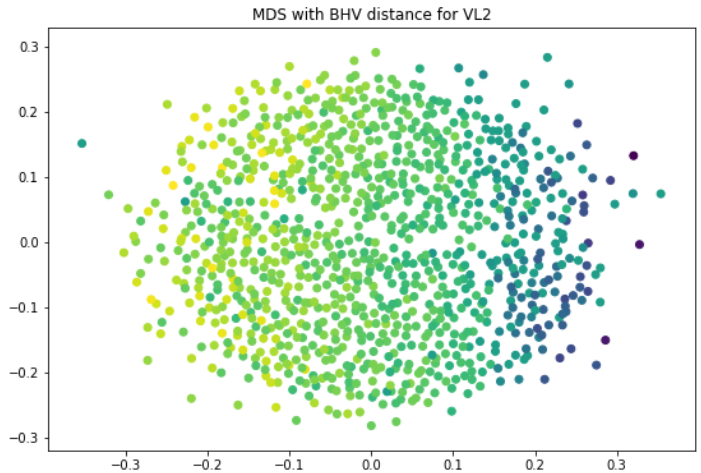
Examples

Colored by first PCA coordinates:



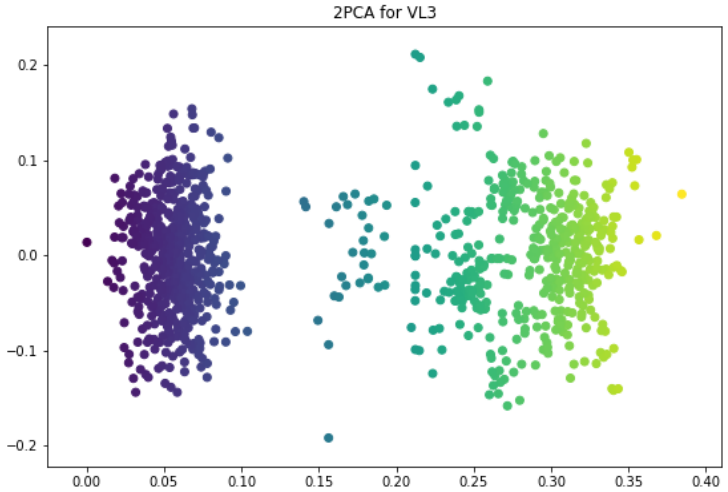


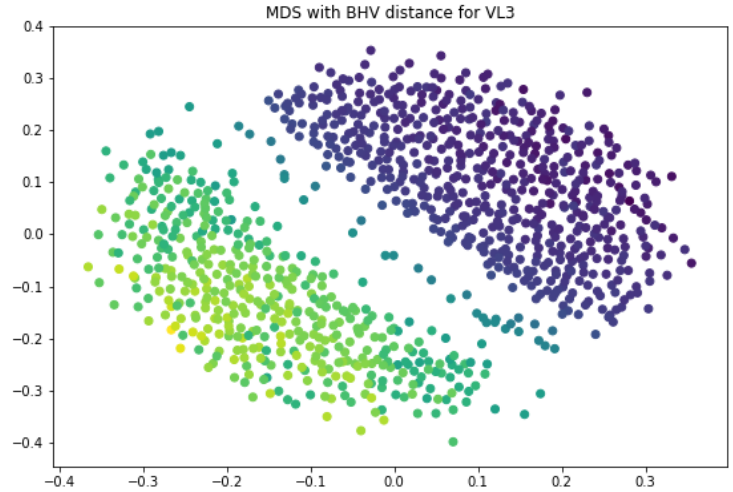


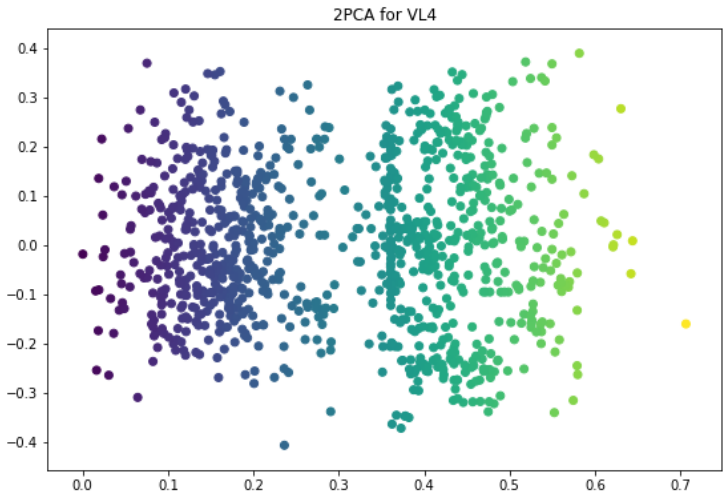


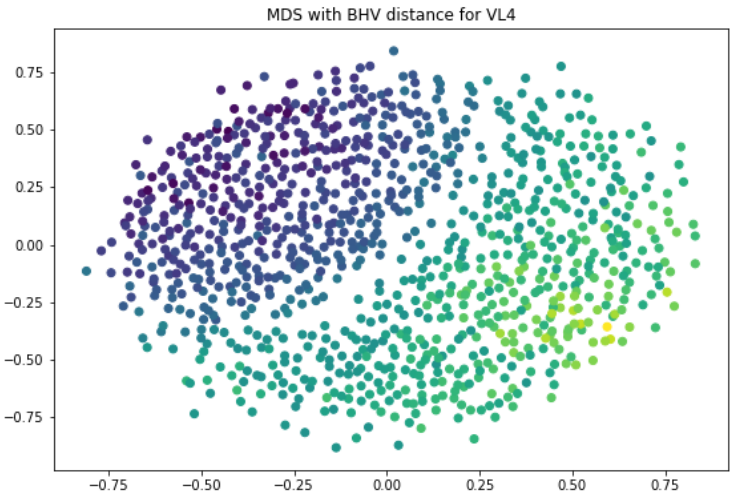
Examples

Colored by first PCA coordinates:







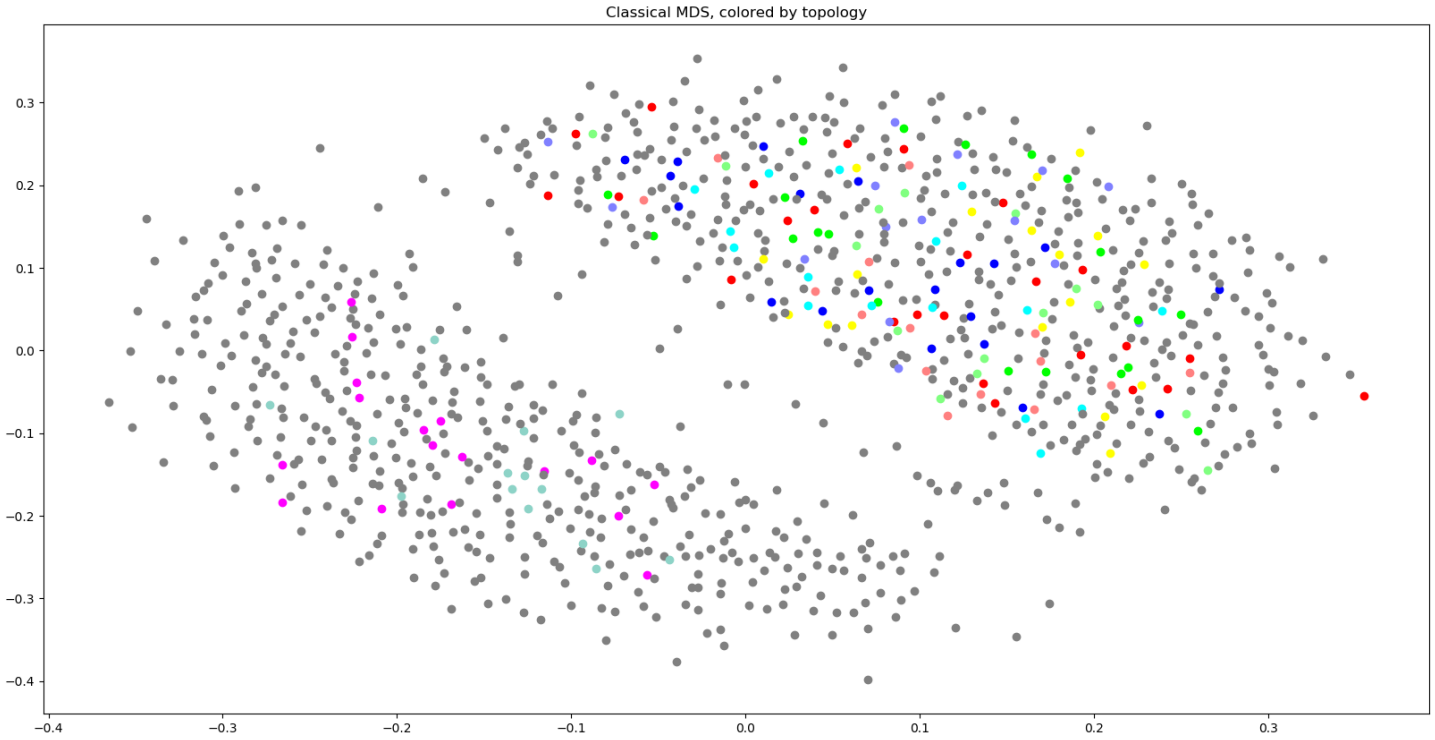


Common topologies in 2PCA

VL3 dataset, Tree PCA colored by topology:

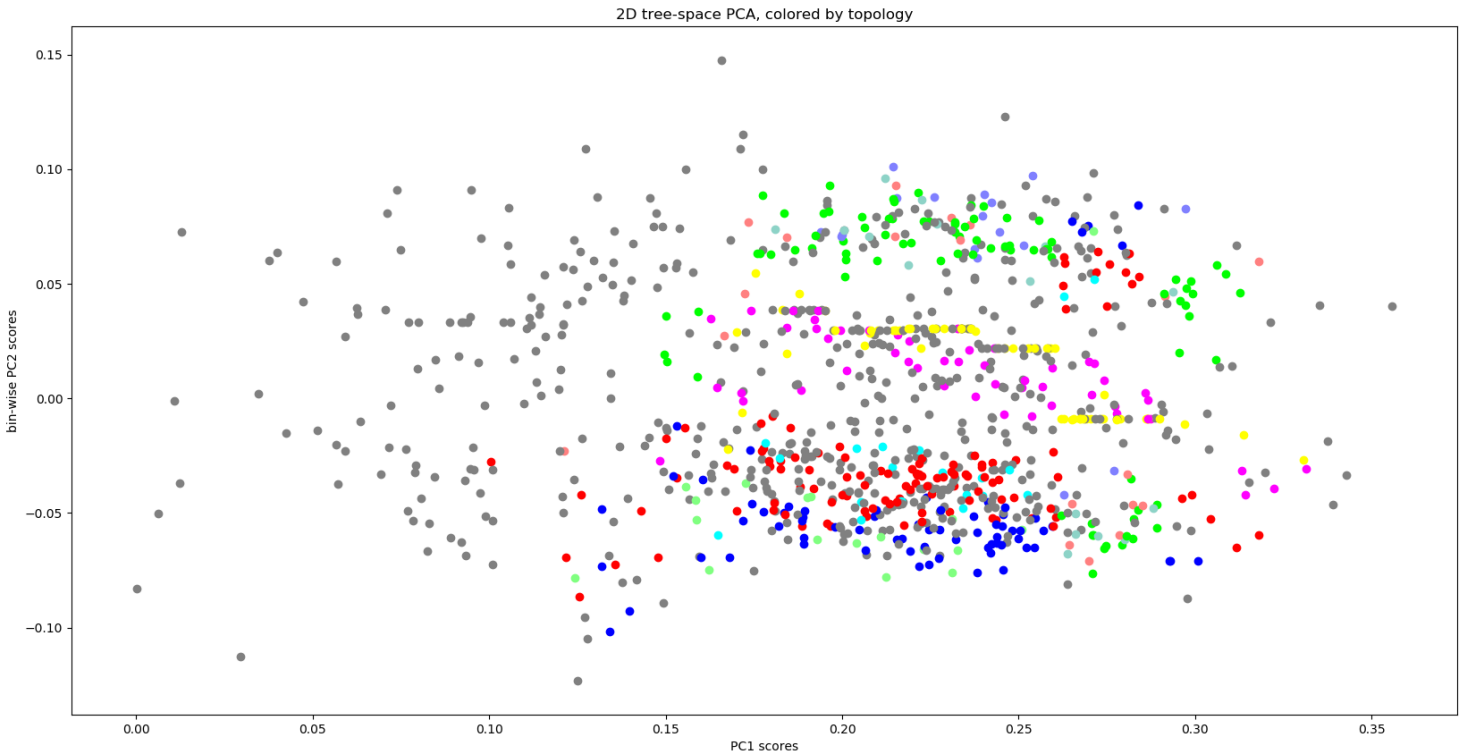
Common topologies in MDS

VL3 dataset, MDS, colored by topology:

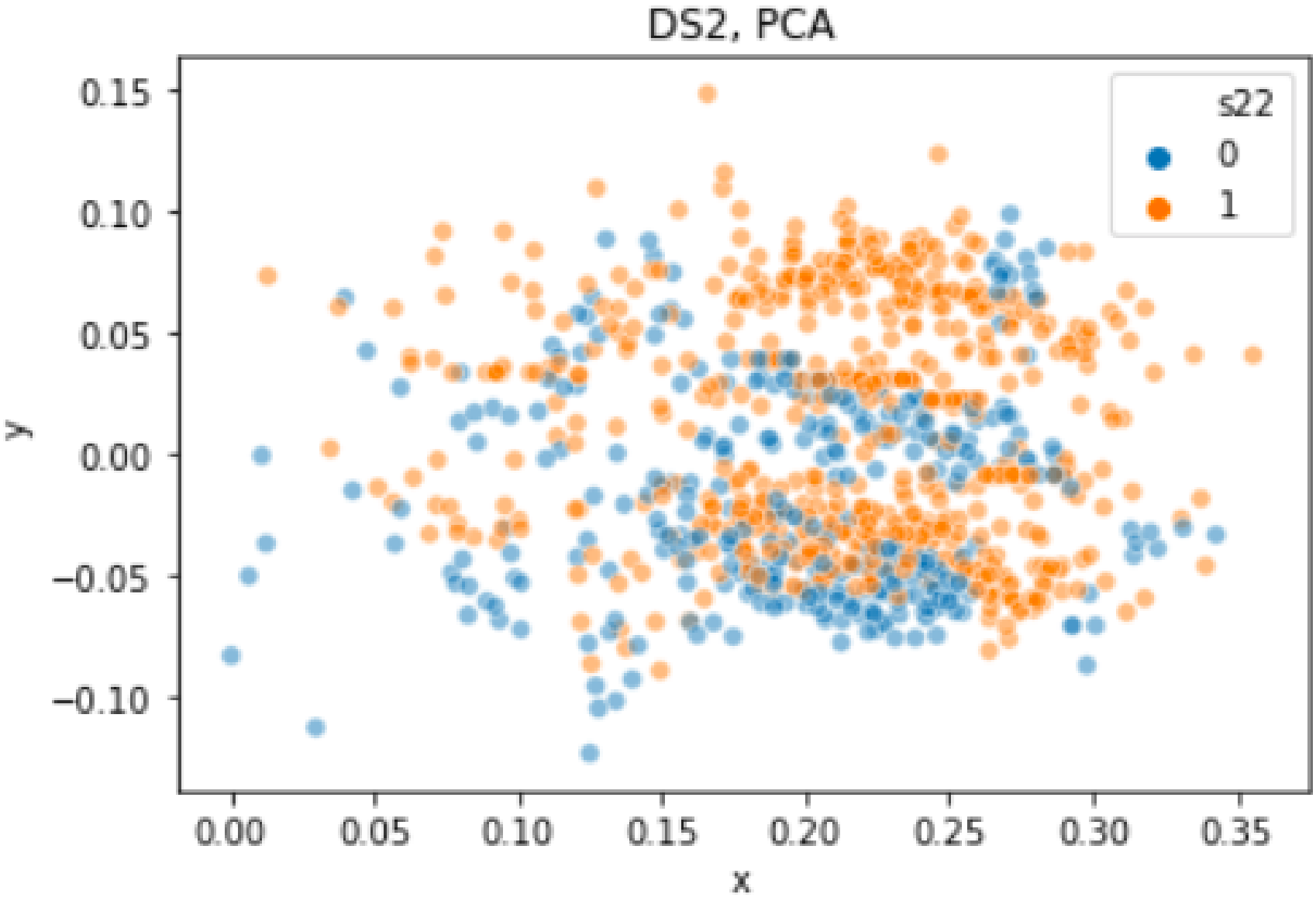


Common topologies in Tree PCA

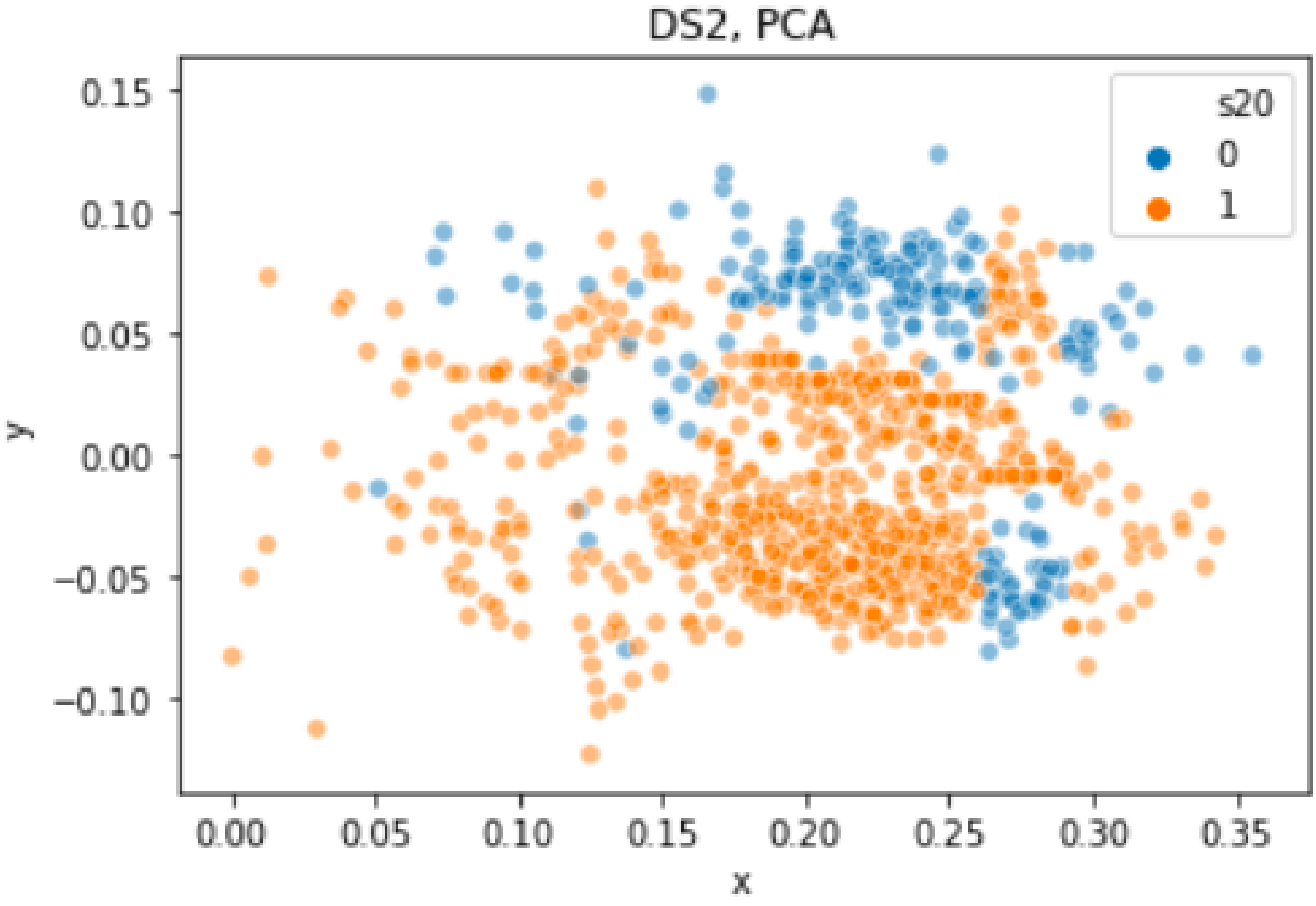
DS2 dataset: 2520 trees on 29 taxa, rDNA; 18s Garey et al. (2012) , sequences from eukaryote species, colored by topology:



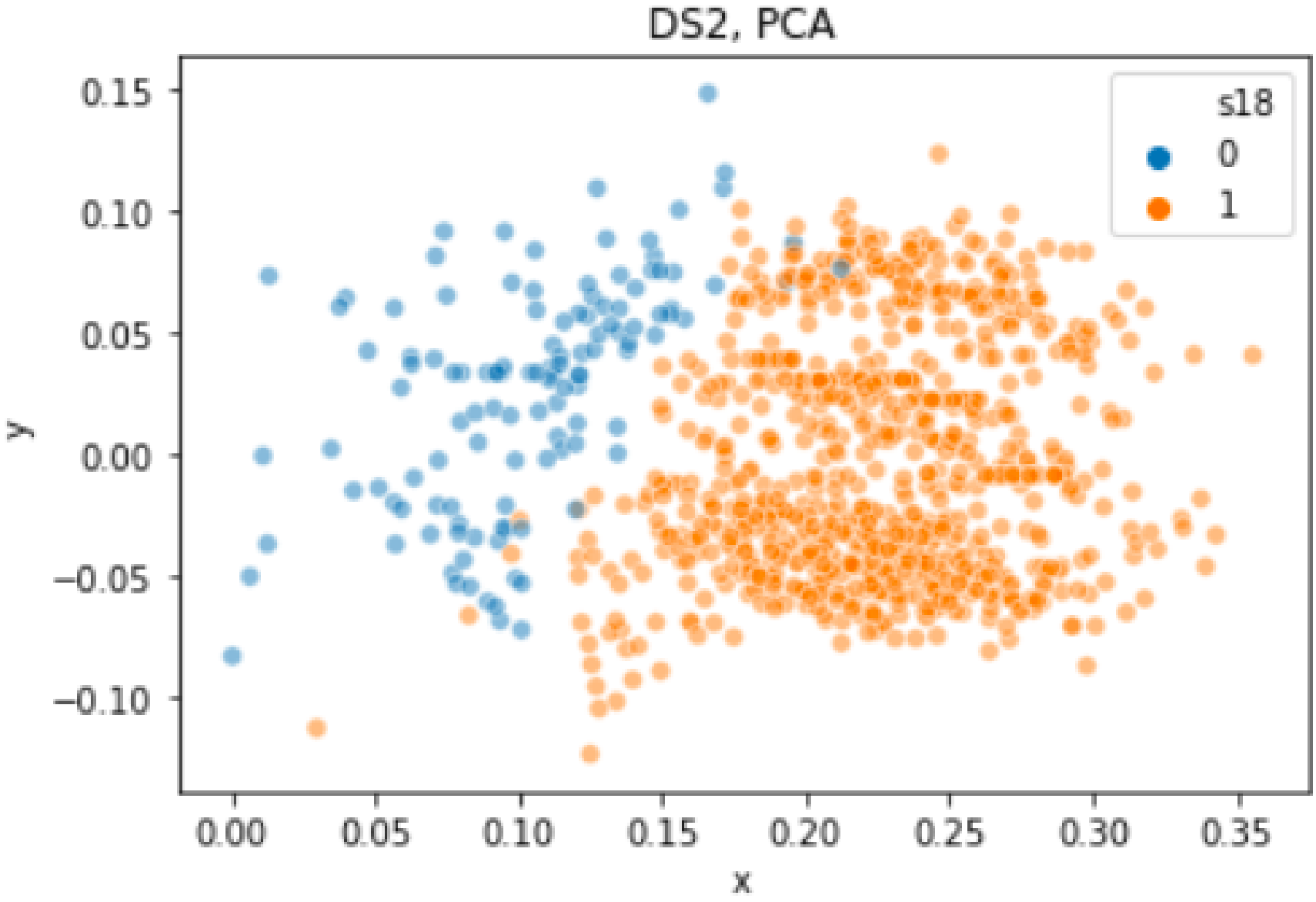
Specific splits: edge 22 present



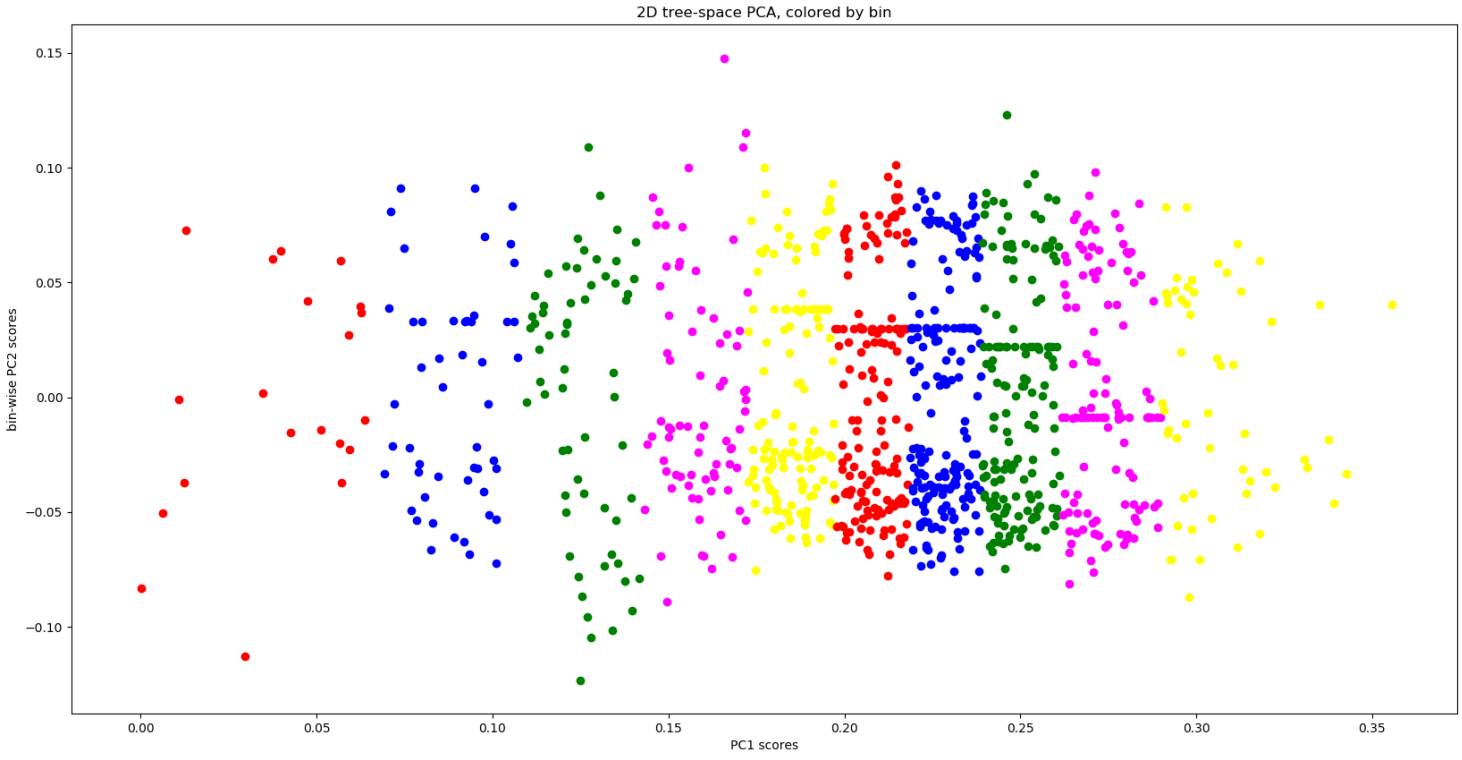
Specific splits: edge 20 present



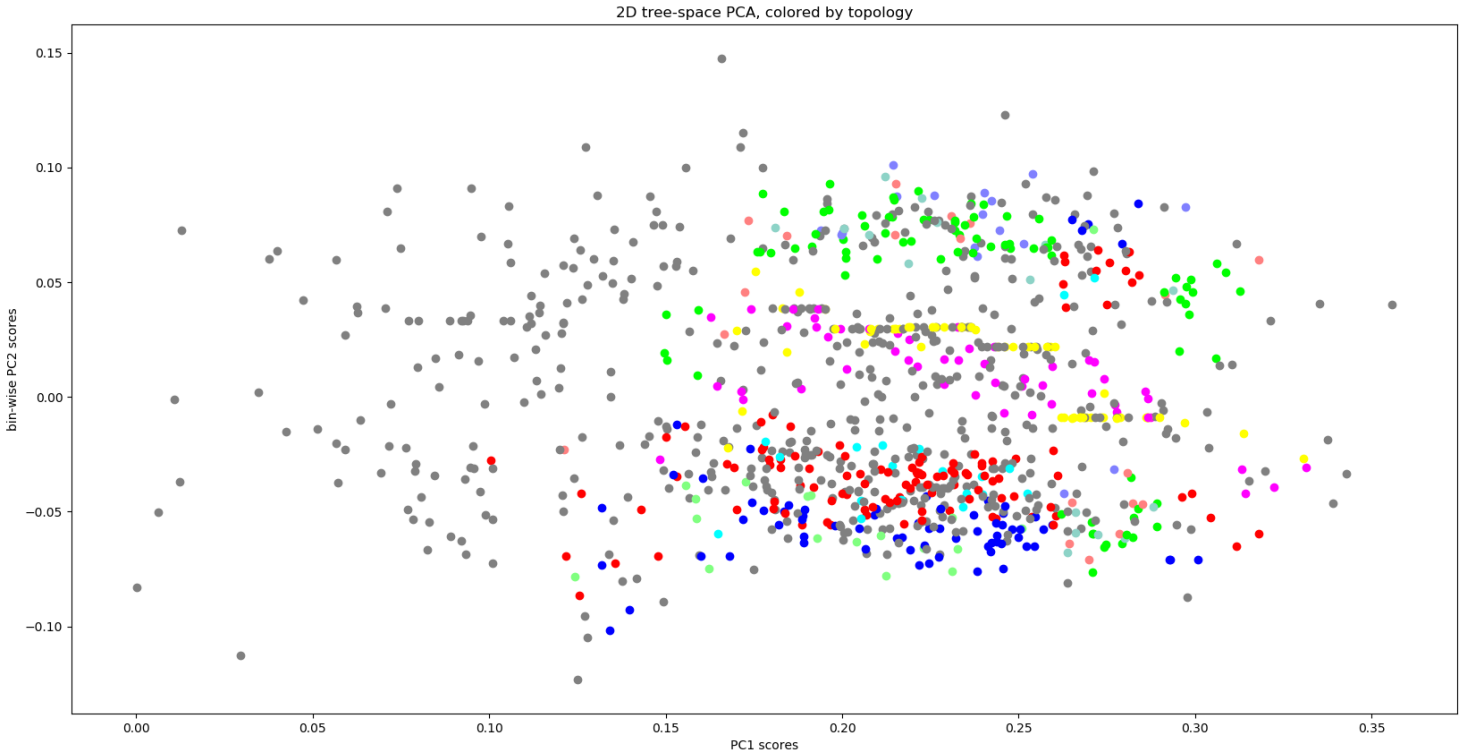
Specific splits: edge 18 present



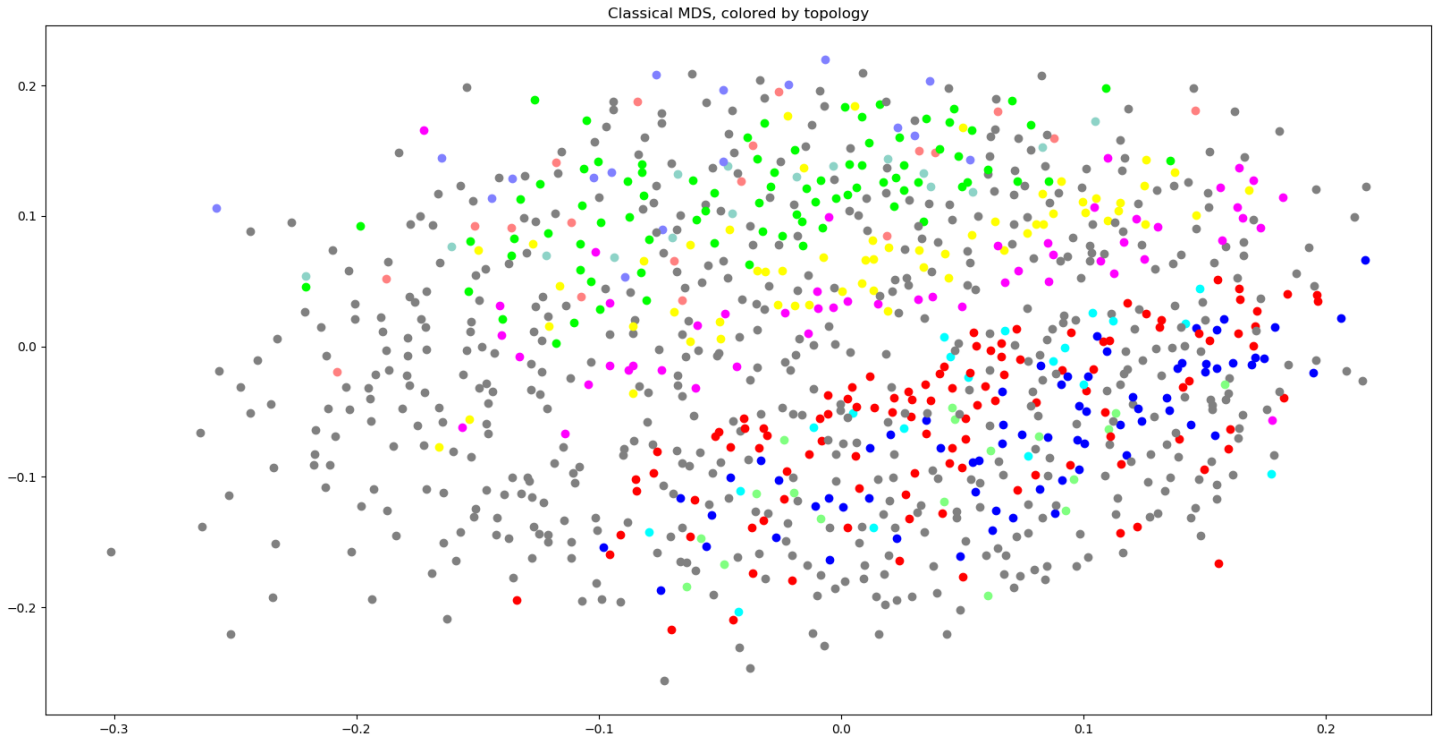
DS2 by bin


2D tree-space PCA, colored by bin
bin-wise PC2 scores
PC1 scores
0.15
0.10
0.05
0.00
−0.05
−0.10
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35

DS2 by topology



DS2 by topology



Observations:

Observations and concerns:

- Number of bins: preset or selected by KDE methods
- Danger of overfitting with many bins
- No guarantee second PCA is perpendicular to first PCA
- Third PCA generally sparse data to fit

Contributors

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Megan Owen: 

Treespace Working Group:

`sites.google.com/site/treespaceworkinggroup/`