# Principal component analysis in treespace

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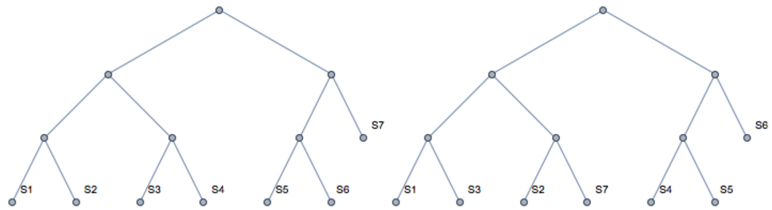
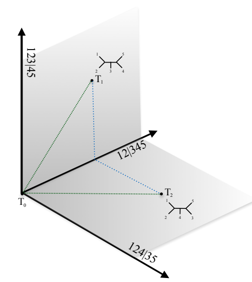
# Distances between phylogenetic trees

- 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) $\Delta$, Subtree-Prune-Regraft (SPR), Tree Bisection and Reconnection (TBR), Billera-Holmes-Vogtmann (BHV), ...

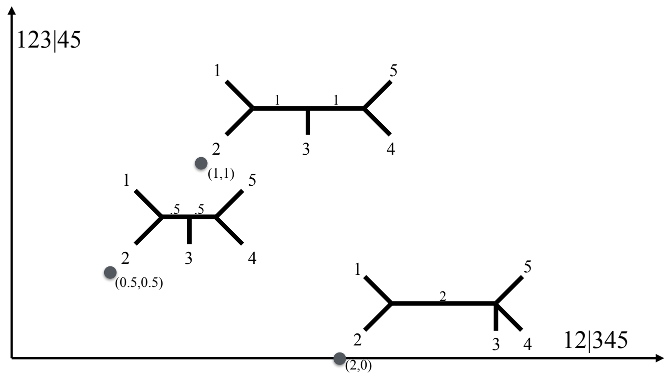
# Trees as Vectors




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

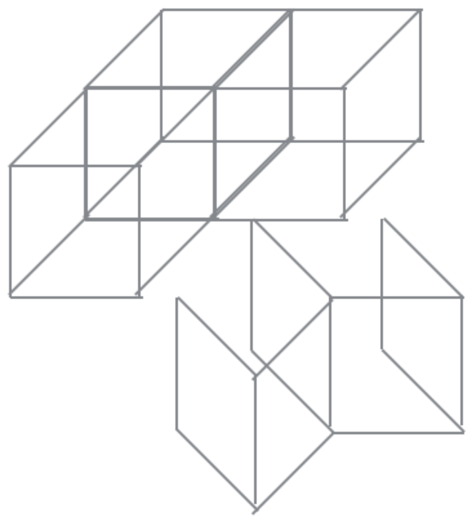
## Billeara-Holmes-Vogtmann space

- 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



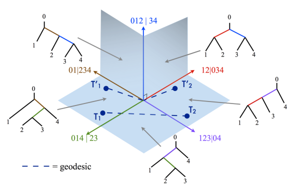
## Billera-Holmes-Vogtmann treespace

- 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



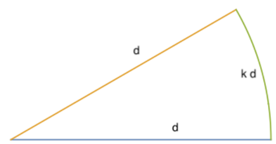
## Finding geodesics in treespace

- 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, ...

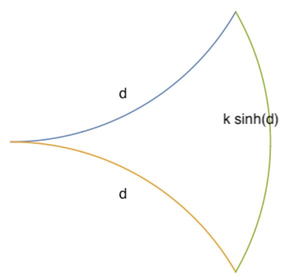


## Divergence of geodesics in hyperbolic space

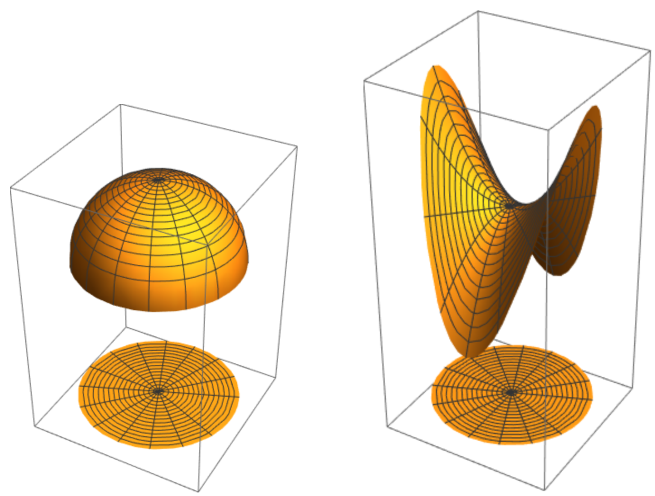
Euclidean: lengths of paths between points on two geodesic rays from $X$ at angle $\theta$ at distance $d$ increases linearly in $d$:




Hyperbolic: lengths of paths between points on two geodesic rays from $X$ at angle $\theta$ 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 $\gamma$ where projections via BHV onto $\gamma$ 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 $\gamma$ the geodesic best capturing the projected distances, parameterize via $[0, 1]$.
- For each $T_i$, find point on $\gamma$ 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 $S_{j,k,\dots}$

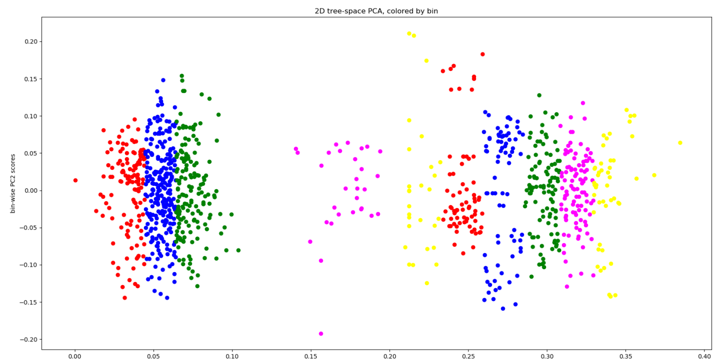
## Two dimensional case

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

- Find $\gamma$, backbone of the entire collection
- Bin trees into say 10 subsets along projections onto $\gamma$
- Find $\gamma_0$ to $\gamma_9$, geodesics for those 10 subsets
- Give coordinates $(x, y)$ to trees based upon their projections onto $\gamma$ and the relevant $\gamma_i$
- Use these coordinates to plot and visualize data

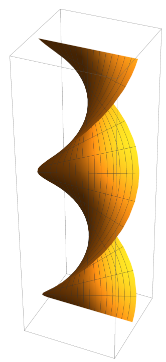
# Example

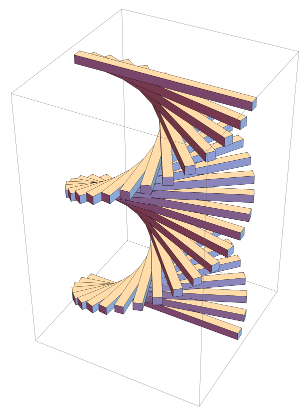
VL3 dataset: 442 trees on 50 taxa, GARTFase Beiko et al. (2006), alignments bacterial and archaeal sequences of protein-coding genes



## Piecewise approximation

Approximate helicoid via backbone and perpendicular parts of changing direction:



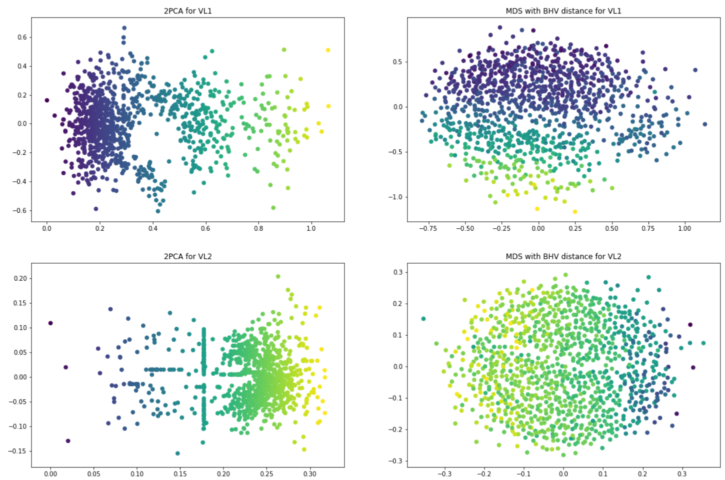


## Properties

- 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

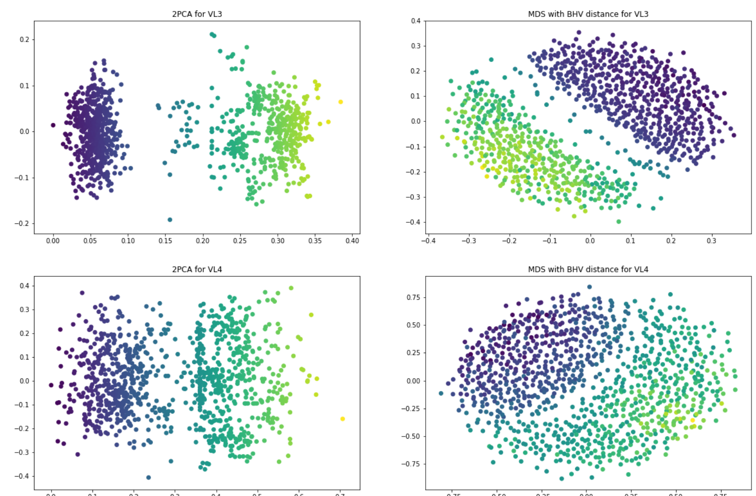
# Examples

Colored by first PCA coordinates:



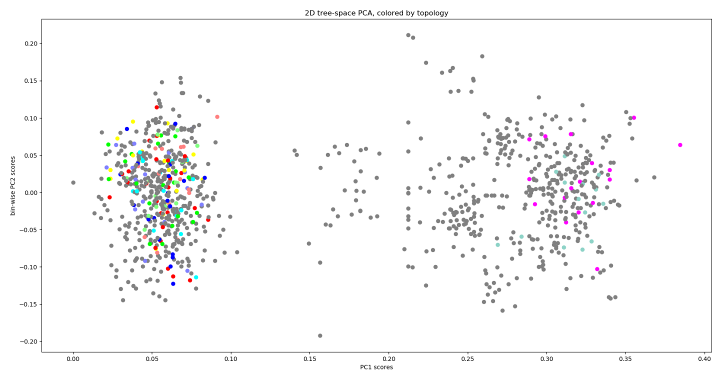
# Examples

Colored by first PCA coordinates:



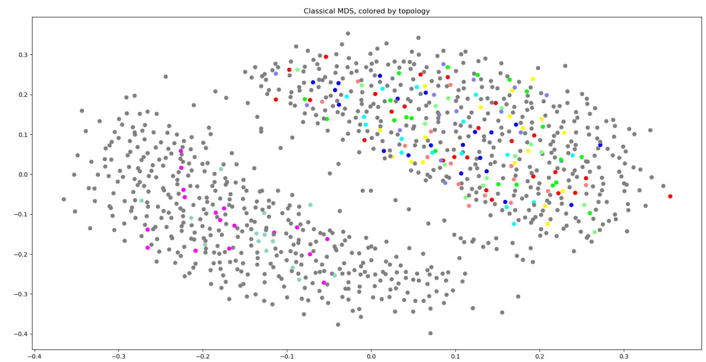
# Common topologies in 2PCA

VL3 dataset, Tree PCA colored by topology:



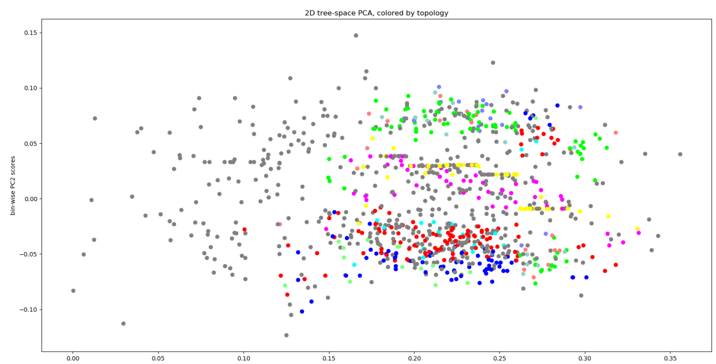
# Common topologies in MDS

VL3 dataset, MDS, colored by topology:

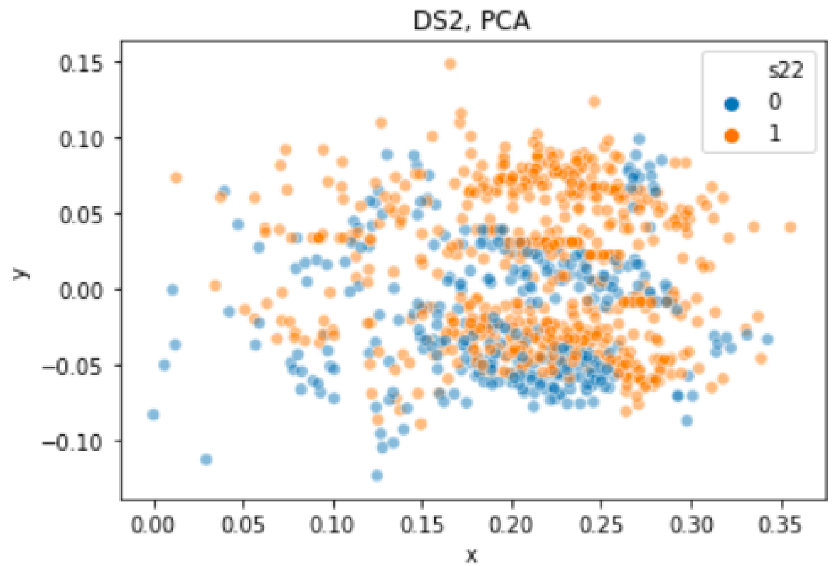


# Common topologies in Tree PCA

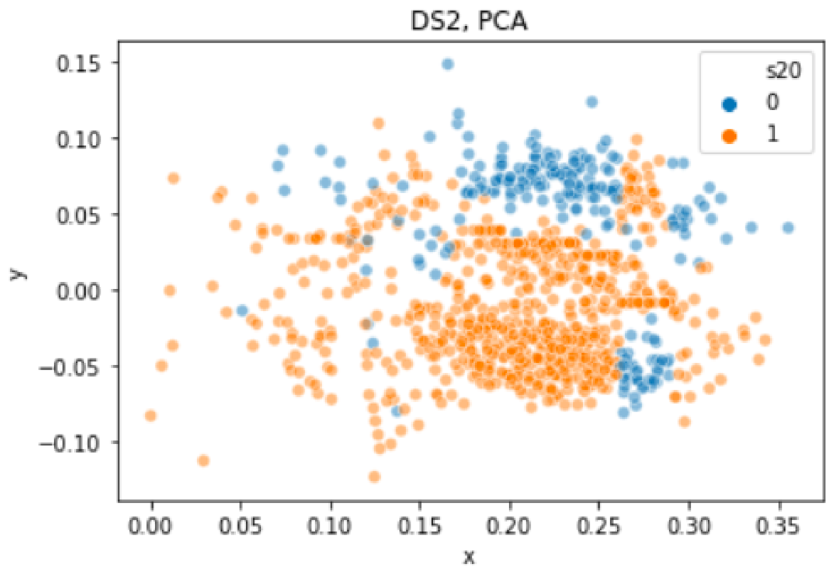
DS2 dataset: 2520 trees on 29 taxa, rDNA; 18s Garey et al. (2012) , sequences from eukaryote species, colored by topology:



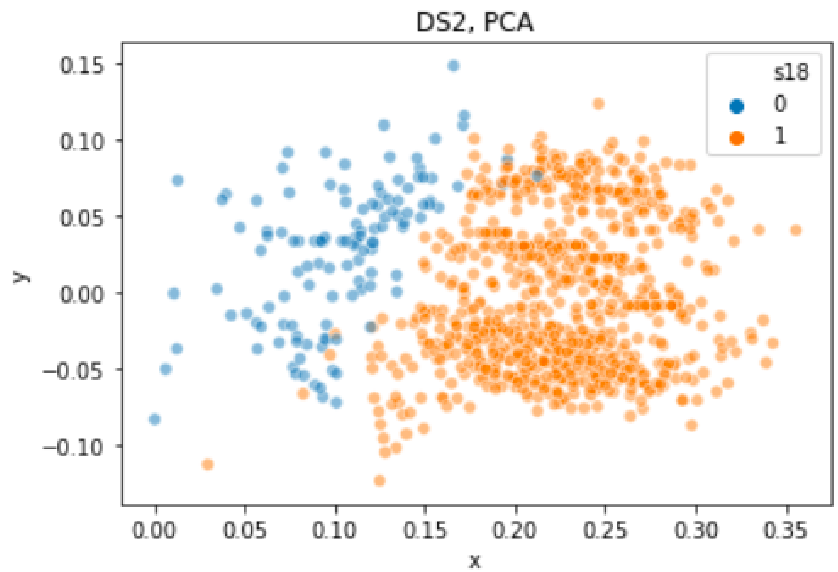
## Specific splits: edge 22 present



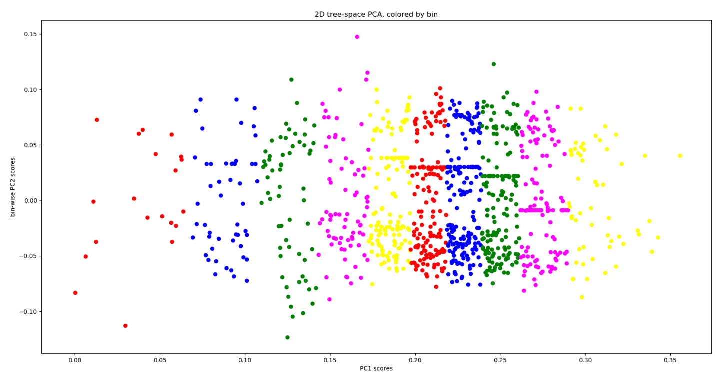
# Specific splits: edge 20 present



## Specific splits: edge 18 present

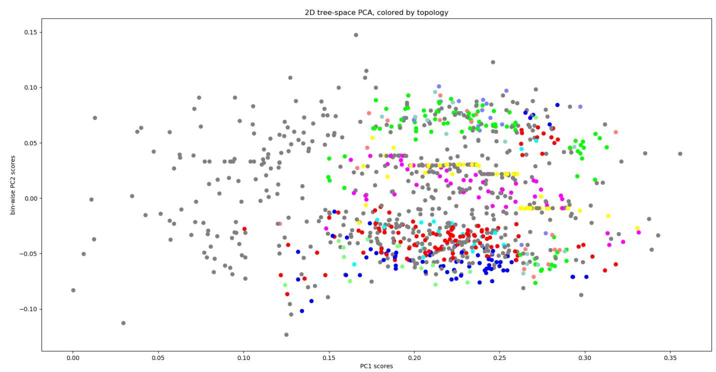


# DS2 by bin

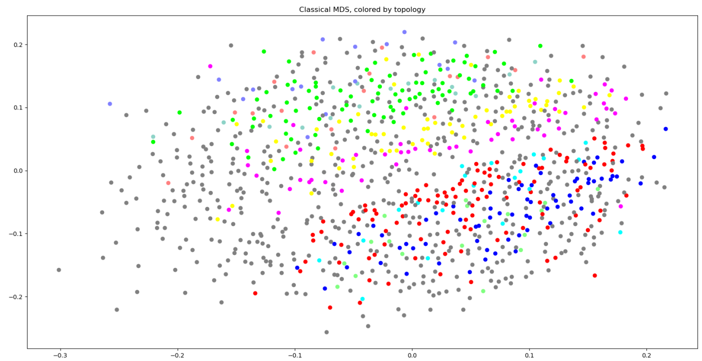


2D tree-space PCA, colored by bin
0.15
0.10
0.05
0.00
−0.05
−0.10
bin-wise PC2 scores
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
PC1 scores

# 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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Treespace Working Group:

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