Exploratory Data Analysis for Data Objects on a Metric Space via Tukey's Depth

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Joint work with Sara Lopez-Pintado

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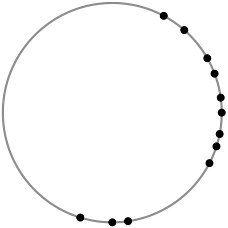
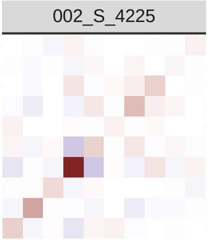
- Brain connectivity in Alzheimer's disease patients
- Phylogenetic trees of parasite species

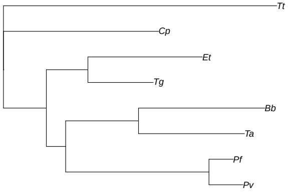
Non-standard data objects



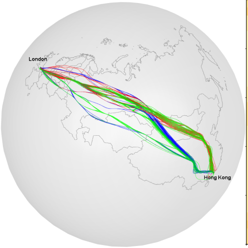
Directions



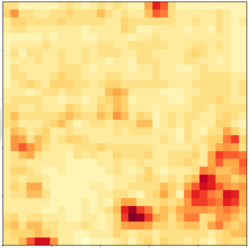
Covariance Matrices



Trees



Functions

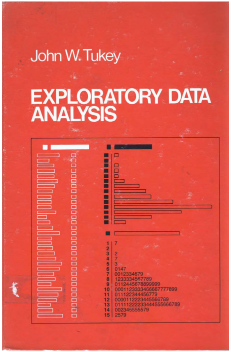


Images

Exploratory data analysis

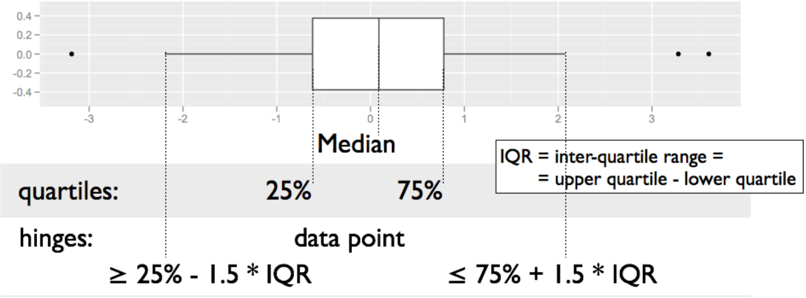
It is important to understand what you CAN DO before you learn to measure how WELL you seem to have DONE it

Exploratory data analysis is detective work



Tukey (1977)

Quantiles in exploratory data analysis



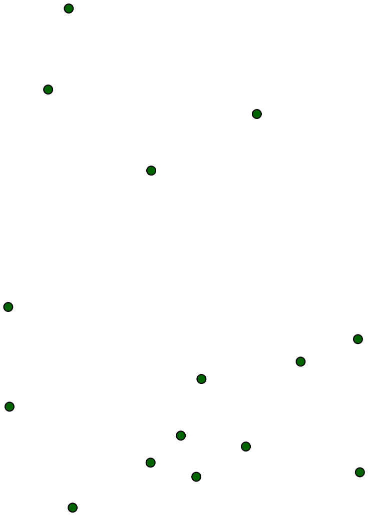
- Quantiles highlight central and extreme data points
- E.g., boxplot for *univariate data*
- Relies on a total ordering
- However, *multivariate data* do not have a canonical ordering

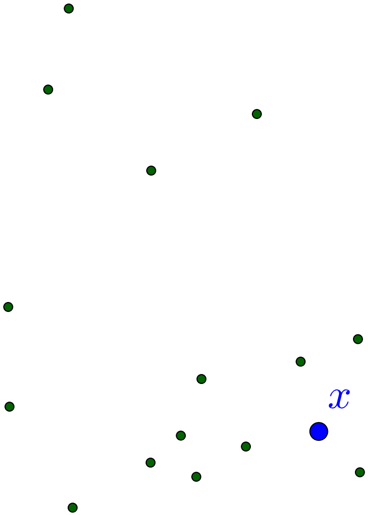
Tukey's depth

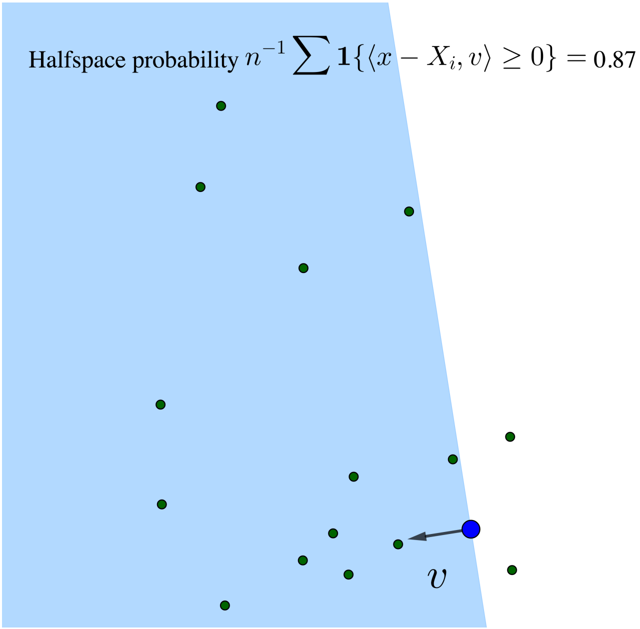
Idea: Measures the "depth", or the centrality of a point relative to a distribution (Tukey, 1975)

- I.i.d. sample $X_1, \ldots, X_n \sim X \in \mathbb{R}^m$
- Tukey's depth of x w.r.t. the sample is

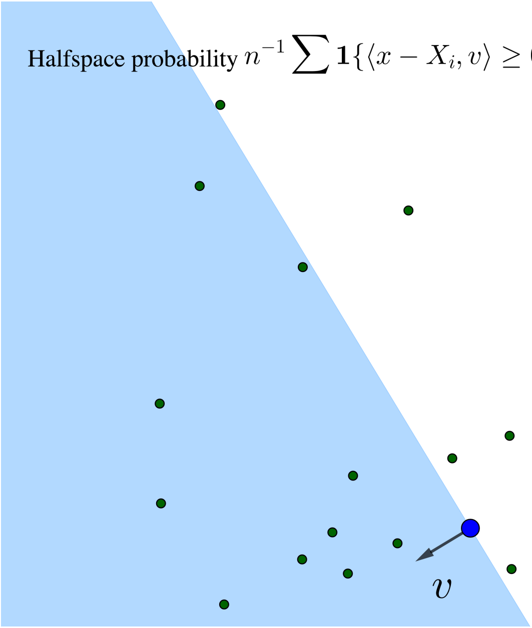
$$D_{\mathrm{Tukey}}(x; P_n) = \inf_{\|v\|=1} \frac{1}{n} \sum_{i=1}^{n} \mathrm{I}\{\langle X_i - x, v \rangle \geq 0\}$$



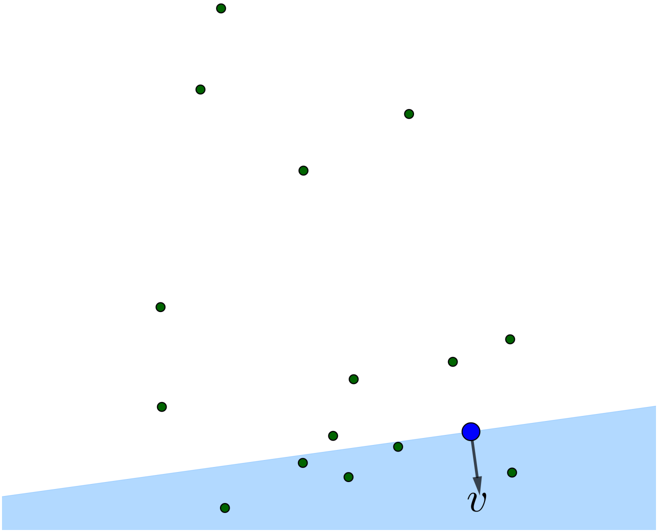

x


Halfspace probability $n^{-1}\sum \mathbf{1}\{\langle x - X_i, v\rangle \geq 0\} = 0.87$
v

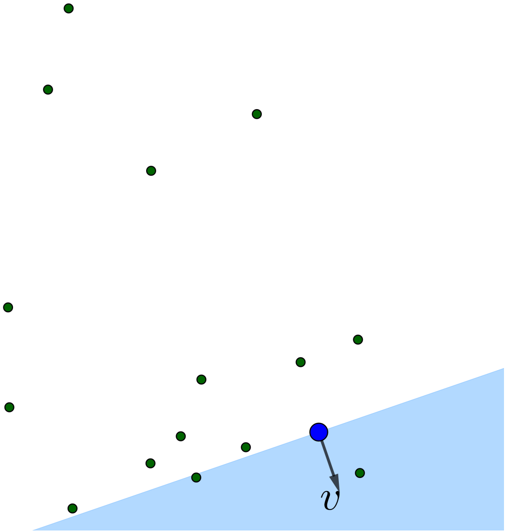
Halfspace probability $n^{-1}\sum \mathbf{1}\{\langle x - X_i, v\rangle \geq 0\} = 0.67$



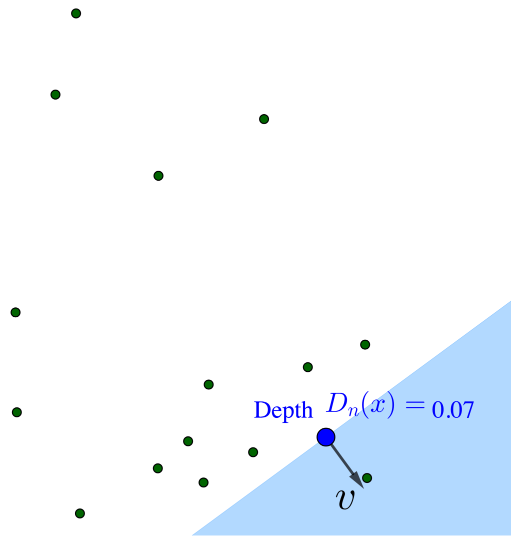
Halfspace probability $n^{-1}\sum \mathbf{1}\{\langle x - X_i, v\rangle \geq 0\} = 0.33$

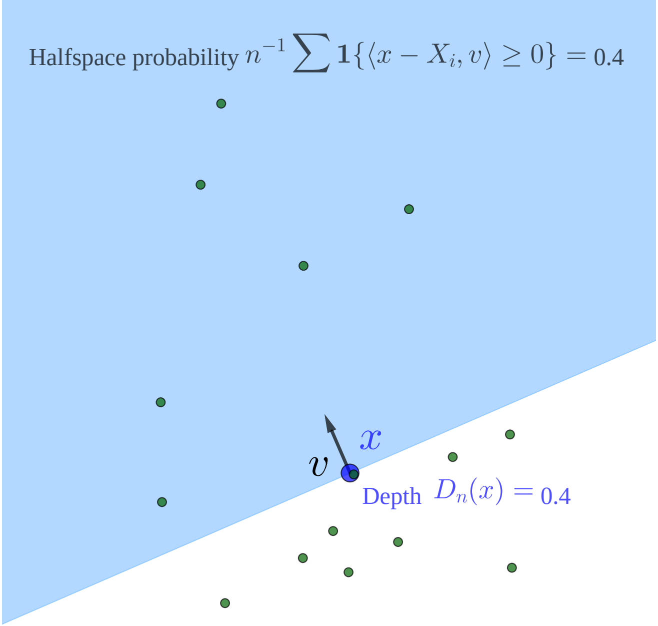


Halfspace probability $n^{-1}\sum \mathbf{1}\{\langle x - X_i, v\rangle \geq 0\} = 0.13$



Halfspace probability $n^{-1} \sum \mathbf{1}\{\langle x - X_i, v \rangle \geq 0\} = 0.07$




Halfspace probability $n^{-1}\sum \mathbf{1}\{\langle x - X_i, v\rangle \geq 0\} = 0.4$
x
v
Depth $D_n(x) = 0.4$

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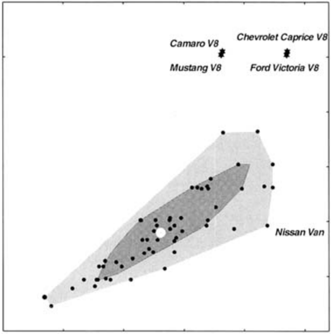
Tukey's depth, cont.

- Measures the centrality/representativeness
- Tukey's depth of $x \in \mathbb{R}^m$ w.r.t. the population is

$$D_{\text{Tukey}}(x; P_X) = \inf_{\|v\|=1} P(\langle X - x, v \rangle \geq 0)$$

- Equals the least probability of any halfspace containing x
- A.k.a halfspace depth
- For univariate data, $D_{\text{Tukey}}(x; P_X) = \min\{F_X(x), 1 - F_X(x)\}$
- Nonparametric
- Differs from densities, which measure the local probability mass
- Deepest point $\theta = \arg\max_{x \in \mathbb{R}^m} D_{\text{Tukey}}(x; P_X)$ is called a depth median
- More generally, Tukey's depth defines a central-outward ranking and quantiles for multivariate data

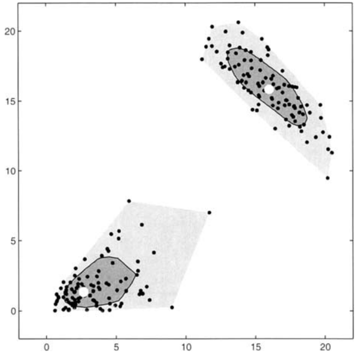
Usage of Tukey's depth: Bagplot (Rousseeuw et al., 1999)



- A bagplot is a bivariate generalization of a boxplot
- From the center outward:
  - The depth median
  - the bag (50% of data)
  - the fence (separates inliers and outliers)
  - outliers

More usage of depth

- Classification (Li et al., 2012)
- Two- or multi-sample inference (Liu and Singh, 1993; Chenouri and Small, 2012)



Multivariate quantile literature

- Only to name a few popular depth functions...
  - Mahalanobis depth (Mahalanobis, 1936)
  - Oja depth (Oja, 1983)
  - Simplicial depth (Liu, 1990)
  - Projection depth (Donoho and Gasko, 1992)
  - Spatial depth (Chaudhuri, 1996; Serfling, 2002)
  - Zonoid depth (Koshevoy and Mosler, 1997)
  - L^p depth (Zuo and Serfling, 2000)
- Transportation approach (Chernozhukov et al., 2017; del Barrio et al., 2020)
- Copula approach (Cousin and Di Bernardino, 2013)

Why does Tukey's depth stand out

Tukey's depth $D_{\mathrm{Tukey}}(\cdot; P_X)$ enjoys nice properties (Donoho and Gasko, 1992; Zuo and Serfling, 2000; Kong and Zuo, 2010):

- Affine invariance
- Maximality at the symmetric center
- Center-outward monotonicity
- Vanishing at infinity
- Robustness
- (Semi-)continuity
- Convexity and compactness of the upper level sets
- Characterizes a certain class of distributions

The first four properties are formulated as desirable for any depth functions (Zuo and Serfling, 2000).

Unfortunately, the computation is very slow for dimension ≥ 4.

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Metric Halfspace Depth

- $(\mathcal{M}, d)$: a metric space
- X: a random element taking values on $\mathcal{M}$
- (Metric) halfspace $H_{x_1x_2} = \{y \in \mathcal{M} \mid d(y, x_1) \leq d(y, x_2)\}$, said to be anchored at $(x_1, x_2) \in \mathcal{M} \times \mathcal{M}$
- Metric halfspace depth w.r.t. the probability measure P_X:

$$D(x) = D(x; P_X) := \inf P_X(H_{x_1x_2}) = \inf P(d(X, x_1) \leq d(X, x_2)).$$

  The infimums are taken over all halfspaces $H_{x_1x_2}$ containing x, i.e., those with $d(x_1, x) \leq d(x_2, x)$
- Metric halfspace depth w.r.t. the sample $X_1, \ldots, X_n$ is

$$D_n(x) = D(x; P_n) := \inf P_n(H) = \inf \frac{1}{n} \sum_{i=1}^{n} \mathrm{I}\{d(X_i, x_1) \leq d(X_i, x_2)\}$$

Metric Halfspace Depth

$$D(x) = \inf_{\substack{x_1, x_2 \in \mathcal{M} \\ d(x_1, x) \le d(x_2, x)}} P(d(X, x_1) \le d(X, x_2))$$

- If $\mathcal{M} = \mathbb{R}^m$, we will recover the Tukey's depth
- In general, the geometry & halfspaces in $\mathcal{M}$ is captured by the distance metric d
- $D(x)$ measures how central/representative x is w.r.t. the distribution
- Data are ranked according to their depth values
- Quantiles can be defined from the rank

Metric Halfspace Depth: Interpretation

$$D(x) = \inf_{\substack{x_1, x_2 \in \mathcal{M} \\ d(x_1, x) \le d(x_2, x)}} P(d(X, x_1) \le d(X, x_2))$$

In the context of social choice,

- Each point in $\mathcal{M}$ is an ideology
- Voters prefer proposals close in ideology
- x, X: Voters
- x_1, x_2: Proposals
- Halfspace probability $P(d(X, x_1) \le d(X, x_2))$: proportion of votes won by x_1 against x_2
- Depth $D(x)$: the minimal popularity attached to a proposal that may appeal to x

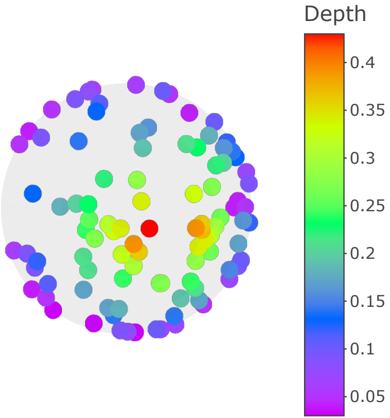
Example: Sphere

Let $\mathcal{M}$ be the unit sphere $\mathbb{S}^m = \{x \in \mathbb{R}^{m+1} \mid x^\intercal x = 1\}$ with the great arc distance $d(x, y) = \arccos(x^T y)$.

- Each metric halfspace $H_{x_1 x_2} = \{y \in \mathcal{M} \mid d(y, x_1) \leq d(y, x_2)\}$ is a closed hemisphere

- The metric halfspace depth recovers the angular Tukey's depth (Small, 1987; Liu and Singh, 1992)

Example: Sphere

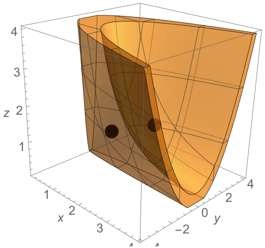


- Depth is monotone from center outward

Example: Symmetric Positive Definite Matrices

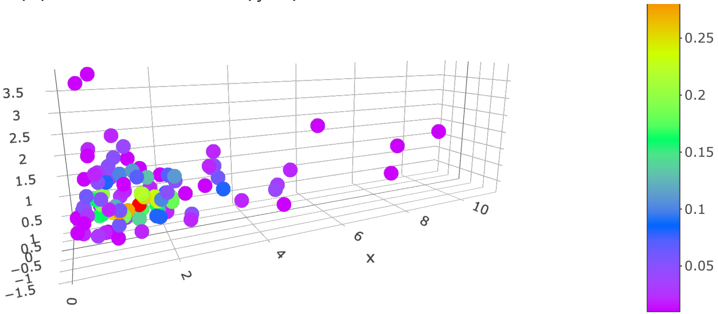
Let $\mathcal{M} = \mathrm{SPD}(k)$ be the manifold of $k \times k$ symmetric positive definite (SPD) matrices.

- Distance: $d(P, Q) = \left\| \mathrm{logm}(P^{-1/2} Q P^{-1/2}) \right\|_F$, where logm is a matrix logarithm
- Affine invariance: $d(APA^\intercal, AQA^\intercal) = d(P, Q)$
- A halfspace in SPD(2) parametrized as $\left(\begin{smallmatrix} x & y \\ y & z \end{smallmatrix}\right)$:



Example: Symmetric Positive Definite Matrices

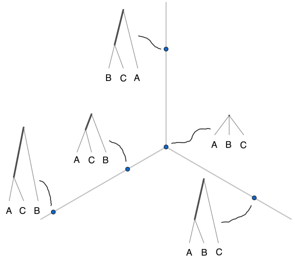
On SPD(2) parametrized as $\begin{pmatrix} x & y \\ y & z \end{pmatrix}$:



- Center-outward
- Reasonable, given large values in the diagonal x, z entries

Example: Trees

Let $\mathcal{M} = \mathbb{T}^k$ be the space of rooted phylogenetic trees with k leaves. Consider $\mathbb{T}^3$ as an example:

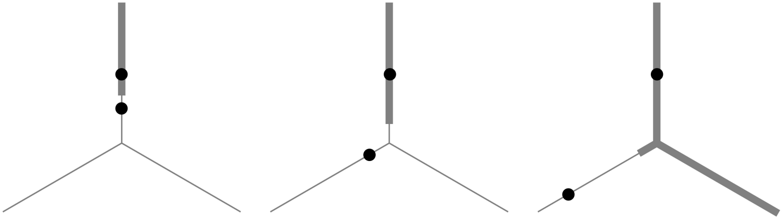


- Each element on $\mathbb{T}^3$ is a phylogenetic tree of three species
- In each tree,
  - Interior node: Speciation event
  - Edge length: Divergence in time or base pairs
- Focus on only the interior edge
- The space $\mathbb{T}^3$ is represented by a 3-spider
  - Branch: Tree topography
  - Location on branch: Length of the interior edge
- In general, $\mathbb{T}^k$ is a cubical complex

Example: Trees

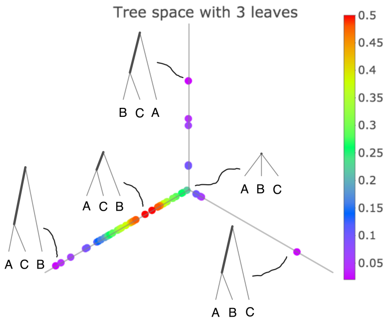
The metric on $\mathbb{T}^k$ is endowed from the Euclidean distance (Billera et al., 2001).

A few halfspaces in $\mathbb{T}^3$:



Example: Trees

Metric halfspace depth:



- Deepest tree occurs around the "center"
- Trees with uncommon topologies have small depth

Related depth literature

- Specialized spaces:
  - unit sphere (Small, 1987; Liu and Singh, 1992)
  - positive definite matrices (Fletcher et al., 2011; Chau et al., 2019)
  - networks (Fraiman et al., 2017)
  - data on a graph (Small, 1997)
  - infinite-dimensional functional data (Fraiman and Muniz, 2001; López-Pintado and Romo, 2009)
- Riemannian manifold: Fraiman et al. (2019)
- General setting: Carrizosa (1996), but only a sketch

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Intuitive depth properties

Depth properties need to be redefined on a non-Euclidean metric space:

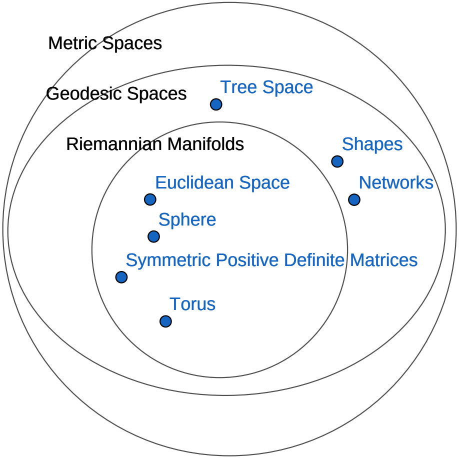
Depth properties in $\mathbb{R}^m$	**Adaptation to $\mathcal{M}$**
Affine invariance	Invariance to halfspace-preserving transformations
Vanishing at infinity	Vanishing at infinite distance from an arbitrary point
Maximality at the symmetrical center	Define halfspace symmetrical distributions
Center-outward monotonicity	Monotonicity along geodesics from the center

Geodesic space and Riemannian manifold

- Let $\gamma : I \to \mathcal{M}$ be a map where I is a closed interval. It is said to be a geodesic if there exists a constant λ such that $d(\gamma(t), \gamma(t')) = \lambda |t - t'|$ for all $t, t' \in I$
- A geodesic joining $x, y \in \mathcal{M}$ is the shortest path between x, y
- $\mathcal{M}$ is a geodesic space if any two points can be joined by a geodesic
- A Riemannian manifold is a smooth submanifold embedded in an ambient Euclidean space
- Riemannian manifolds are special cases of geodesic spaces

Geodesic space and Riemannian manifold

Practically, one can define a metric structure for any data analysis



Intuitive depth properties

Theorem 1

1. *(Transformation invariance) If f is a halfspace invariant transformation at $x \in \mathcal{M}$, then $D(x; P_X) = D(f(x); P_{f(X)})$.*
2. *(Vanishing at infinity) Let $o \in \mathcal{M}$ be an arbitrary point. Then $\sup_{x:d(o,x)>L} D(x) \to 0$ as $L \to \infty$.*
3. *(Maximality at the symmetrical center) If there exists a unique point θ s.t. $P(X \in H) \geq 1/2$ for any halfspace H containing θ, then θ is the unique deepest point.*
4. *(Center-outward monotonicity) Suppose that $\mathcal{M}$ is a geodesic space. Let $\theta \in \mathcal{M}$ be a deepest point, $x \in \mathcal{M}$, and $\gamma : [0,1] \to \mathcal{M}$ a geodesic joining θ to x. If any halfspace $H_{x_1x_2}$ of $\mathcal{M}$ that has a nonempty intersect with $\gamma([0,1])$ contains at least one of x and θ, then $D(x) \leq D(\gamma(t))$ holds for $t \in [0,1]$.*

- The geometric condition for the monotonicity is satisfied by the spheres, Euclidean spaces, and hyperbolic spaces

Depth function and depth region

Define depth regions $D^\alpha := \{x \in \mathcal{M} \mid D(x) \geq \alpha\}$, for $\alpha \geq 0$

Proposition 1

Suppose that $\mathcal{M}$ is a complete and locally compact geodesic space.

1. *$D(\cdot)$ is upper semi-continuous.*
2. *D^α is nested, i.e. $D^{\alpha_1} \subset D^{\alpha_2}$ for $\alpha_1 \geq \alpha_2$, and D^α is compact for $\alpha > 0$.*

Convergence properties

Let $\mathcal{H}$ be the collection of halfspaces in $\mathcal{M}$.

Theorem 2

If the Vapnik–Chervonenkis (VC) dimension of $\mathcal{H}$ is finite, then as $n \to \infty$,

$$\sup_{x \in \mathcal{M}} |D_n(x) - D(x)| = O(n^{-1/2}) \quad a.s.$$

- $\mathbb{S}^m$ and $\mathbb{T}^3$ have finite VC dimension

Let $\theta = \arg\max_{x \in \mathcal{M}} D(x)$ and $\theta_n = \arg\max_{x \in \mathcal{M}} D_n(x)$.

Proposition 2

Under regularity conditions, as $n \to \infty$,

$$d(\theta_n, \theta) \to 0 \quad a.s.$$

Robustness of the depth median

The breakdown point (Donoho and Gasko, 1992) of a statistic

- is a measure of robustness
- is the least proportion of adversarial contamination in the dataset so as to bring the statistic to infinity.
- $\mathcal{X}$: Dataset of n points; $\mathcal{Y}$: contamination set
- For the depth median θ, the breakdown is defined as

$$\epsilon^* = \min \left\{ \frac{n_\epsilon}{n + n_\epsilon} \,\middle|\, \sup_{|\mathcal{Y}| = n_\epsilon} \sup_{p \in \theta(\mathcal{X} \cup \mathcal{Y})} d(X_1, p) = \infty \right\}.$$

- Larger breakdown $\implies$ more robust

Robustness of the depth median

Proposition 3

On any metric space $\mathcal{M}$, it holds that

$$\epsilon^* \geq \frac{D_n(\theta_n)}{1 + D_n(\theta_n)},$$

where θ_n is a depth median w.r.t. sample $\mathcal{X}$.

- $D_n(\theta_n) \to D(\theta)$
- For a halfspace symmetric distribution, breakdown $\epsilon^* \geq 1/3$

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Computation of metric halfspace depth

- Computing a single Tukey's depth value exactly takes $O(n^{m-1} \log n)$ (Dyckerhoff and Mozharovskyi, 2016)
- Optimization on non-Euclidean spaces is hard
- Need efficient approximation

Approximate algorithm

Let $\mathcal{X} = \{X_1, \ldots, X_n\}$ be the observations, and $\mathcal{A} \subset \mathcal{M}$ the anchor set.

- Approximate $D_n(x)$ by

$$\tilde{D}_n(x; \mathcal{A}) = \inf_{\substack{x_1 \neq x_2 \in \mathcal{A} \\ d(x, x_1) \leq d(x, x_2)}} \frac{1}{n} \sum_{i=1}^{n} \mathrm{I}\{d(X_i, x_1) \leq d(X_i, x_2)\}$$

- $\mathcal{A}$ can be set to $\mathcal{X}$
- To improve approximation, enhance $\mathcal{A}$ with jiggled points
- Approximate the depth median using the deepest in-sample observation

$$\tilde{\theta} = \arg\max_{x \in \mathcal{X}} \tilde{D}_n(x)$$

Approximate algorithm

Algorithm 1: Metric Halfspace Depth Algorithm

Data: Depth evaluation points $\mathcal{Y}$, observations $\mathcal{X}$, and anchor set $\mathcal{A}$

Result: Depth values $\tilde{D}_n(y;\mathcal{A})$ for $y \in \mathcal{Y}$

1 For $x_1 \neq x_2 \in \mathcal{A}$, obtain halfspace probabilities $p_{x_1 x_2} = n^{-1} \sum_{i=1}^{n} I\{X_i \in H_{x_1 x_2}\}$

2 For $y \in \mathcal{Y}$, obtain $\tilde{D}_n(y;\mathcal{A}) = \min\{p_{x_1 x_2} \mid d(y, x_1) \leq d(y, x_2), x_1 \neq x_2 \in \mathcal{A}\}$

- Time complexity if $\mathcal{A} = \mathcal{X}$: $O(n_{\mathcal{Y}} n^2 + n^3)$, independent of the dimension
- Depends only on the pairwise distances

Theory for the approximation

Theorem 3

Under regularity conditions, if the infimum in $D(x) = \inf_{H \in \mathcal{H}_x} P(H)$ is achieved by a halfspace, then as $n \to \infty$,

$$\left| \tilde{D}_n(x; \mathcal{X}) - D(x) \right| = O_p(a_n).$$

If the infimum of $D(x) = \inf_{H \in \mathcal{H}_x} P(H)$ is not achieved by any halfspace, then as $n \to \infty$,

$$\left| \tilde{D}_n(x; \mathcal{X}) - D(x) \right| = o_p(1).$$

- a_n measures how dense the random sample $\mathcal{X}$ is around the anchors of the minimizing halfspace
- $O_p(a_n) = O_p(n^{-1/m})$ on an m-dimensional Riemannian manifold

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Simulation studies

- Target: Estimate the center μ of a symmetrical distribution on $\mathcal{M}$
- Our proposal: Deepest point $\hat{\mu}_{\mathrm{MHD}}$
- Competitors:
  - Fréchet mean $\hat{\mu}_{\mathrm{FM}} = \arg\min_{x \in \mathcal{M}} \sum_{i=1}^{n} d(x, X_i)^2$, non-robust; Fréchet (1948)
  - Fréchet median $\hat{\mu}_{\mathrm{GDD}} = \arg\min_{x \in \mathcal{M}} \sum_{i=1}^{n} d(x, X_i)$, robust; Chau et al. (2019)
- Metric: $d(\hat{\mu}, \mu)$
- Goal: Compare efficiency and robustness

Results on $SPD(k)$

	$n =$	$k=2$ MHD	$k=2$ FM	$k=2$ GDD	$k=3$ MHD	$k=3$ FM	$k=3$ GDD	$k=4$ MHD	$k=4$ FM	$k=4$ GDD
No contamination	50	.118	.102	.120	.122	.102	.121	.110	.102	.121
	100	.076	.070	.075	.071	.070	.077	.076	.070	.077
	200	.054	.052	.049	.055	.051	.050	.056	.051	.050
Location contamination	50	.119	.143	.132	.109	.147	.115	.111	.144	.115
	100	.097	.122	.104	.084	.119	.088	.087	.133	.096
	200	.077	.110	.085	.062	.108	.071	.062	.109	.078
Scale contamination	50	.091	.104	.102	.098	.104	.092	.102	.103	.092
	100	.074	.075	.072	.060	.076	.068	.061	.075	.066
	200	.058	.057	.054	.043	.055	.051	.038	.054	.051
Loc & scale contamination	50	.123	.143	.128	.114	.150	.111	.115	.144	.119
	100	.096	.127	.107	.086	.125	.092	.082	.130	.092
	200	.067	.112	.087	.057	.115	.072	.058	.112	.076

Results on $\mathbb{S}^k$ and SO(k)

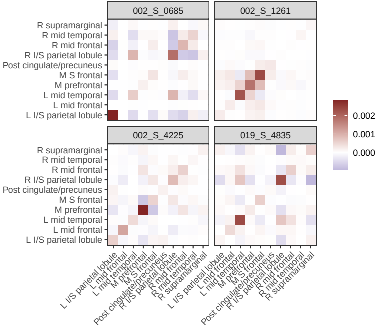
		$\mathcal{M} = \mathbb{S}^k$						$\mathcal{M} = \mathrm{SO}(k)$					
		$k=2$		$k=3$		$k=4$		$k=2$		$k=3$		$k=4$	
	$n=$	MHD	FM	MHD	FM	MHD	FM	MHD	FM	MHD	FM	MHD	FM
No contam	50	.146	.124	.147	.131	.142	.131	.113	.093	.116	.107	.127	.107
	100	.090	.092	.101	.093	.096	.093	.071	.065	.082	.076	.092	.076
	200	.066	.066	.069	.067	.072	.068	.048	.048	.084	.054	.072	.054
Location contam	50	.146	.137	.165	.164	.146	.171	.128	.111	.142	.150	.140	.149
	100	.111	.126	.123	.147	.105	.142	.086	.084	.119	.129	.096	.123
	200	.093	.117	.087	.120	.092	.122	.093	.097	.118	.110	.097	.111
Scale contam	50	.126	.132	.127	.151	.125	.154	.113	.093	.114	.113	.106	.110
	100	.098	.096	.092	.102	.083	.107	.071	.065	.085	.082	.073	.082
	200	.073	.067	.072	.078	.057	.080	.048	.048	.077	.062	.062	.057
Loc & scale contam	50	.144	.153	.161	.177	.136	.192	.128	.111	.138	.145	.137	.153
	100	.105	.141	.120	.159	.108	.159	.084	.084	.124	.132	.099	.127
	200	.091	.133	.081	.130	.087	.134	.093	.097	.111	.112	.095	.115

Functional connectivity in Alzheimer's disease patients

- Data from Alzheimer's Disease Neuroimaging Initiative (ADNI)
- Raw data point: fMRI scan
- After preprocessing: Connectivity measure as a 10×10 covariance matrix between 10 regions of interest
- $n = 181$ subjects
- Four groups:
  - cognitively normal (CN)
  - early mild cognitive impaired (EMCI)
  - late mild cognitive impaired (LMCI)
  - Alzheimer's disease (AD)
- Goal: Detect group difference

Functional connectivity in Alzheimer's disease patients

Raw data:

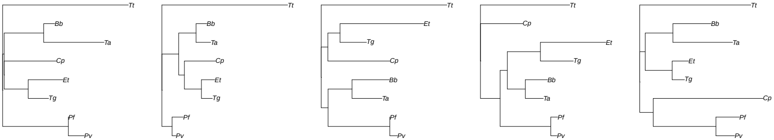


p-values from pairwise depth-based Wilcoxon tests (Chenouri and Small, 2012):

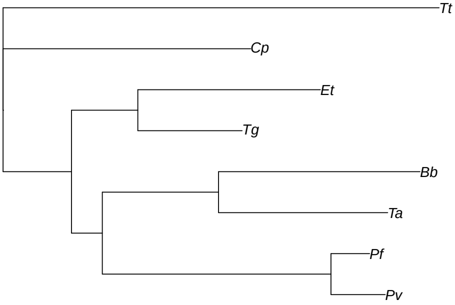
	EMCI	LMCI	AD
CN	0.644	0.339	0.021
EMCI	–	0.350	0.126
LMCI	–	–	0.074

Phylogenetic trees

- Apicomplexan phylogeny (Kuo et al., 2008)
- Data: Phylogenetic trees for 7 species (and 1 outgroup), one tree for each gene
- $n = 268$ genes
- Goal: Find a consensus tree, and detect outliers
- Some tree observations:

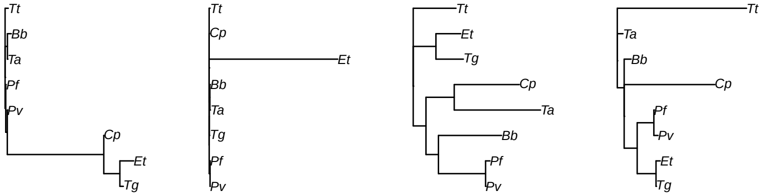


Deepest tree under MHD



- The tree topology of the deepest tree coincides with the best known topology
- No need to identify and remove outliers before analysis
- Monophyletic/siblings which makes sense:
  - *Pf* & *Pv*: Malaria parasites
  - *Bb* & *Ta*: Tick-borne parasites
  - *Et* & *Tg*: Coccidian species

Outlier trees



- Trees with the least metric halfspace depth are potential outliers
- Exceptionally long branches: 1st & 2nd
- Wrong tree topography: 1st, 3rd, & 4th

Takeaways

Metric halfspace depth

- measures the representativeness of data points on a metric space
- leads to intuitive center-outward ranks and quantiles
- shows successes in estimating the center and identifying outliers

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