

Automated Shape Correspondence: *Why and How*

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Outline

- Goals & Rationale
- Limitations of traditional landmarks
- Definition of ‘automated correspondence’ & potential
- Automated approaches and their limitations thus far
- *Auto3dgm*: Concepts & Logistics
- Homology and its relationship to correspondence
- On the horizon

Goals & Rationale

Goal

- To achieve data driven understanding of the pattern of micro- and macroevolution that describes the anatomical diversity of life.

Requirement

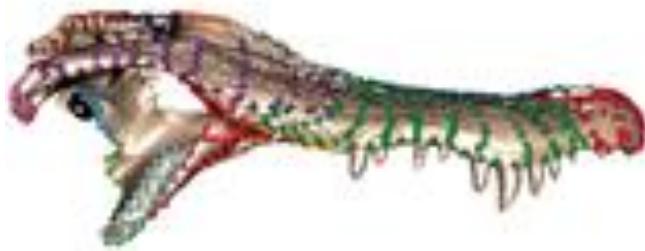
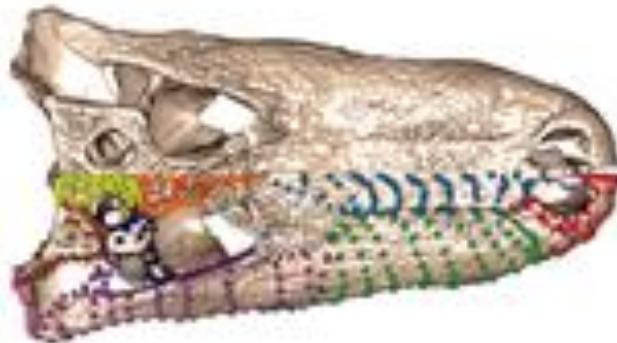
- Quantitative approaches capable of meaningfully aligning and/or comparing “the same organ in different animals under every variety of form and function”

Rationale

- Without such a framework, comparative morphology will remain arbitrarily limited in its ability to quantitatively describe the morphological (and potentially evolutionary) continuity uniting different individuals and species.

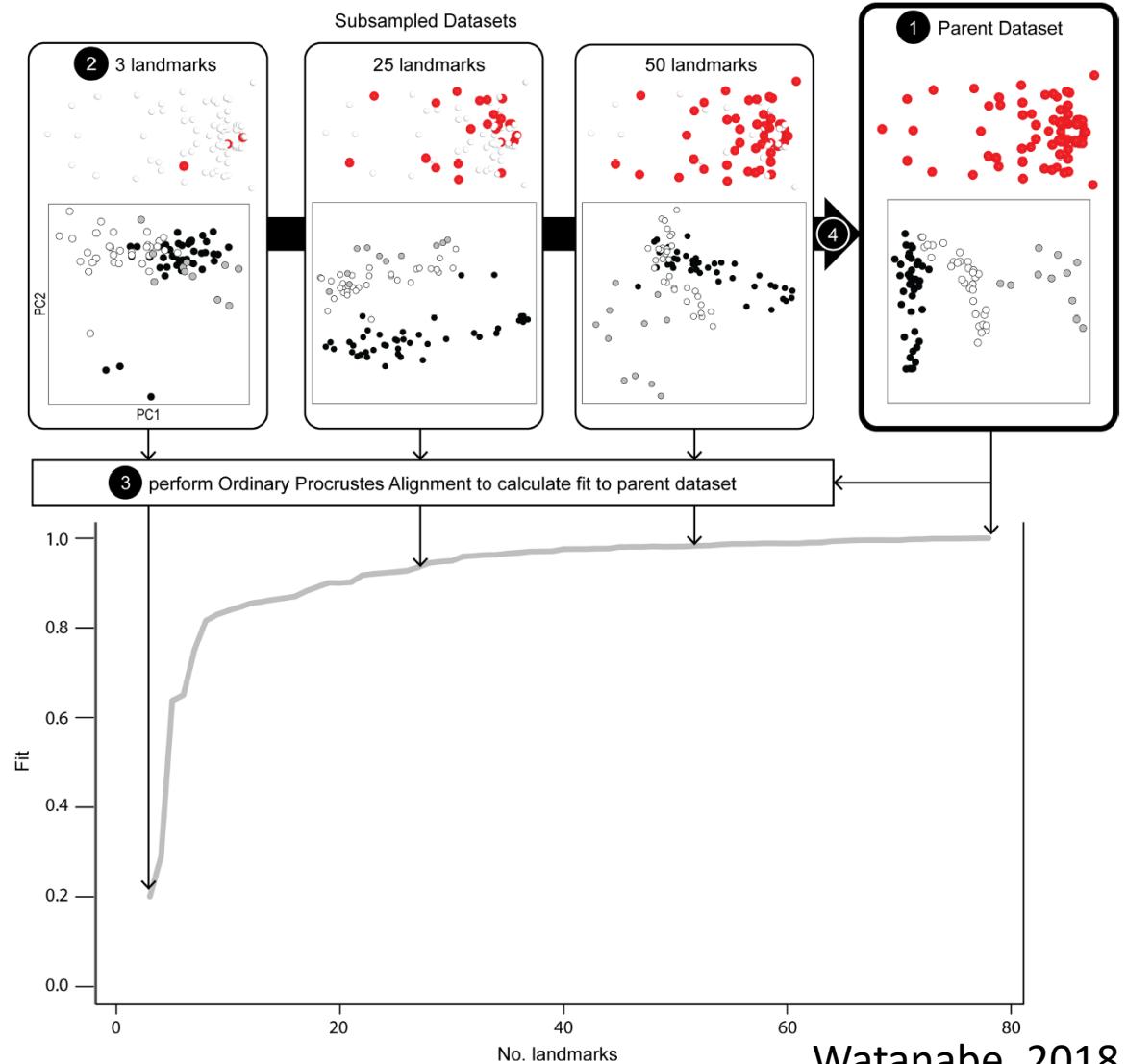
Limitations of traditional landmarks

- 1) Time consuming for richly corresponding shapes
 - Inadequate coverage → instable shape characterization



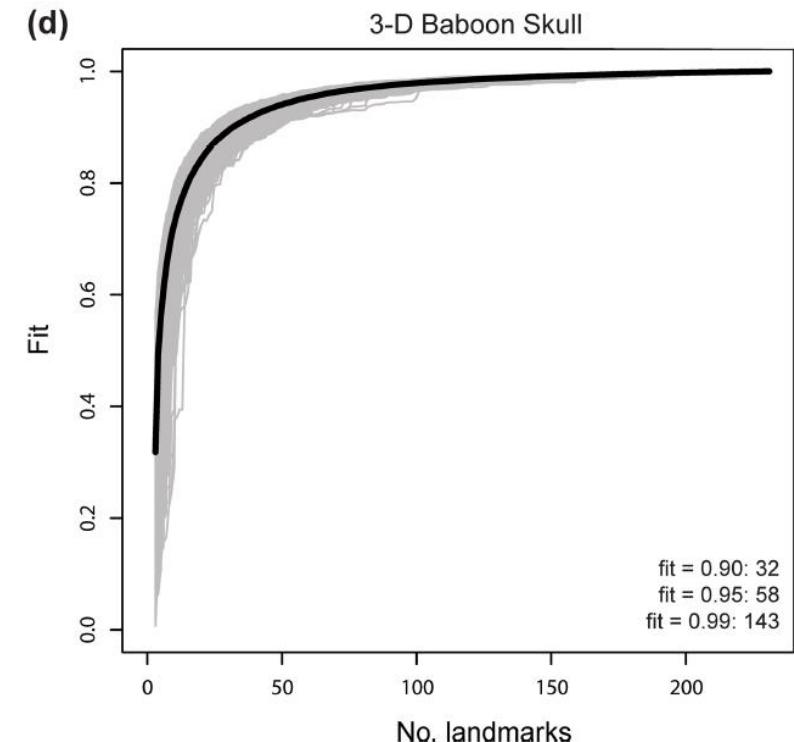
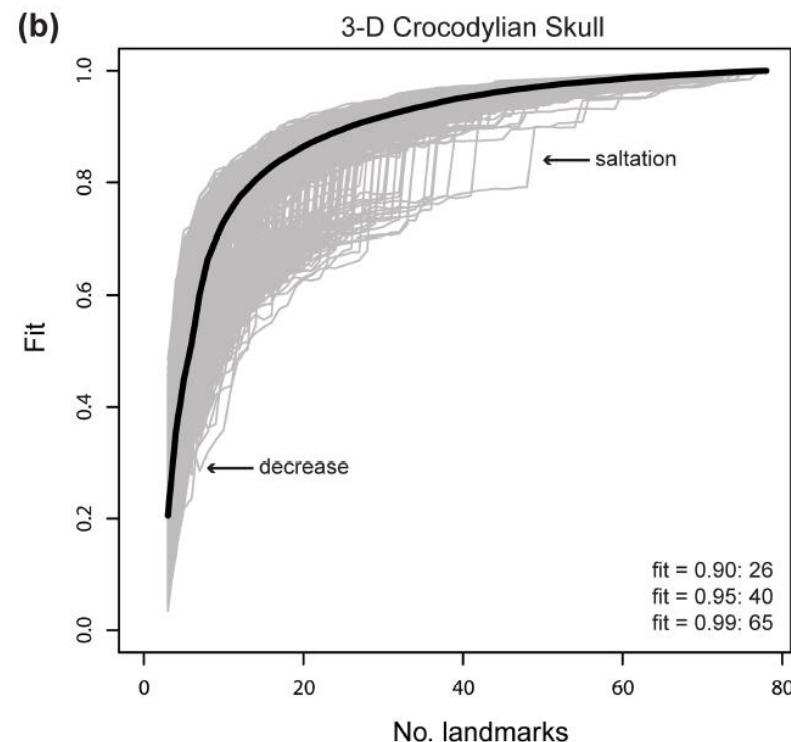
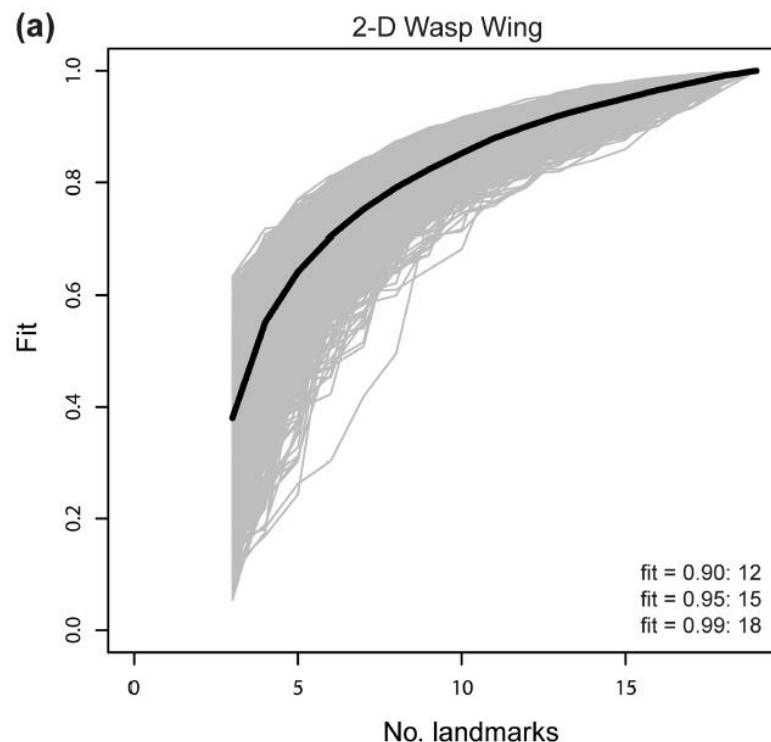
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Limitations of traditional landmarks

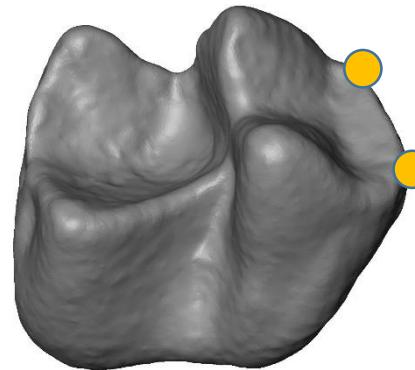
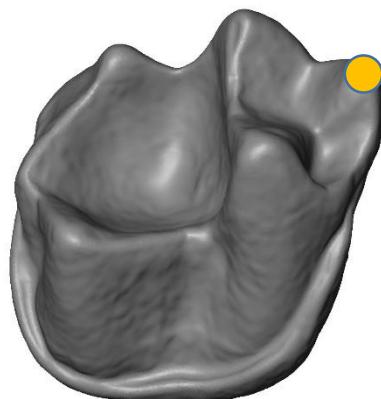
- 1) Time consuming for richly corresponding shapes
 - Inadequate coverage → instable shape characterization



Limitations of traditional landmarks

- 2) Data to represent shape must be chosen *a priori*, maybe subjectively

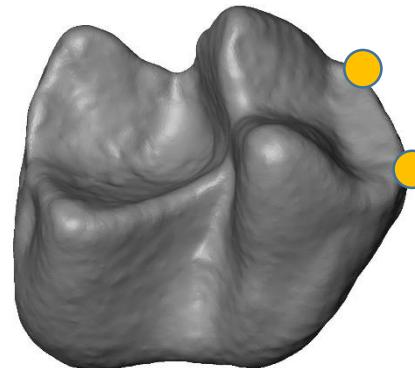
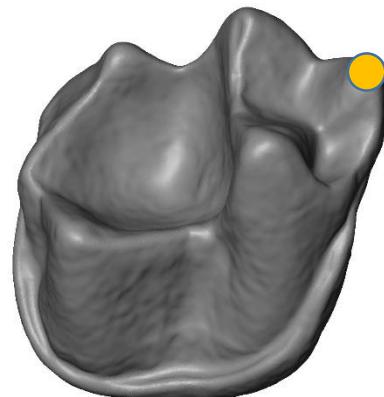
“As a general rule, landmarks should be chosen so you can quantify any differences that you can see” (Zelditch et al., 2004)



?

Limitations of traditional landmarks

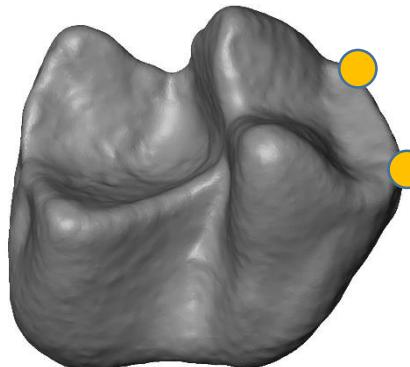
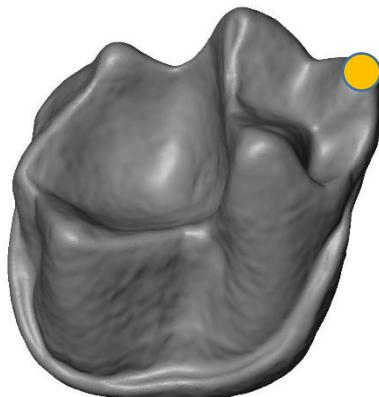
- 3) Criterion of *homology* can be difficult to substantiate in practice
 - Leads to differing interpretations of homologous points
 - Also expressed as inflated inter- or intraobserver error



Limitations of traditional landmarks

4) Cannot be used for “topology” changes

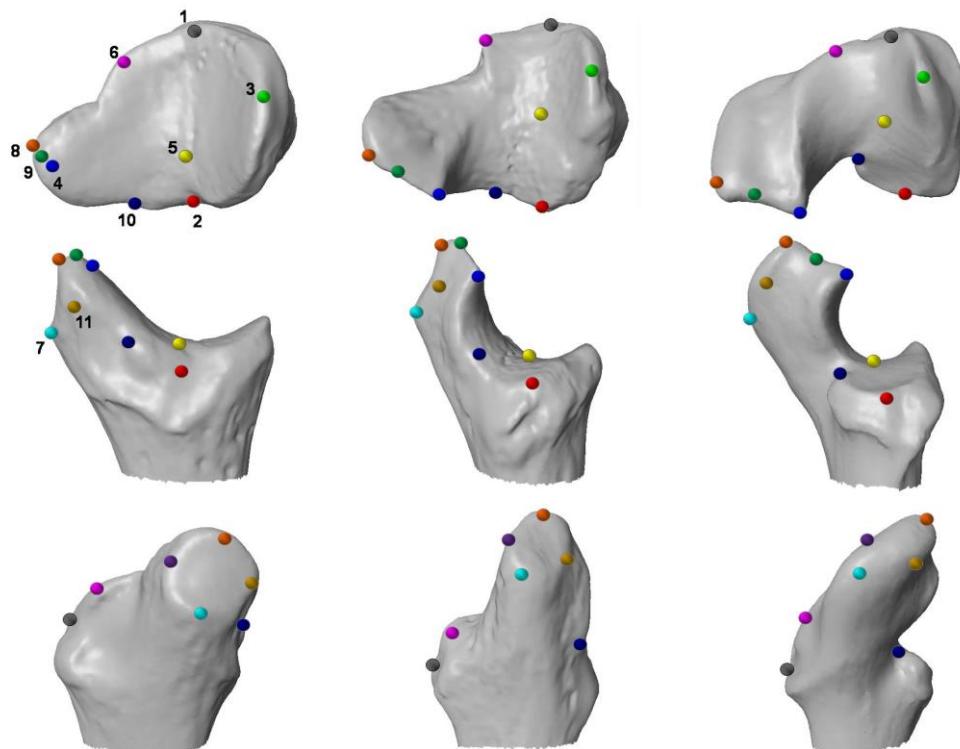
- i.e., differences reflecting missing features will not be quantified (Zelditch et al., 2004)
- *Coverage* will not be adequate (Watanabe, 2018)
 - too few landmarks
 - Landmarks not repeatable



Limitations of traditional landmarks

4) Cannot be used for “topology” changes

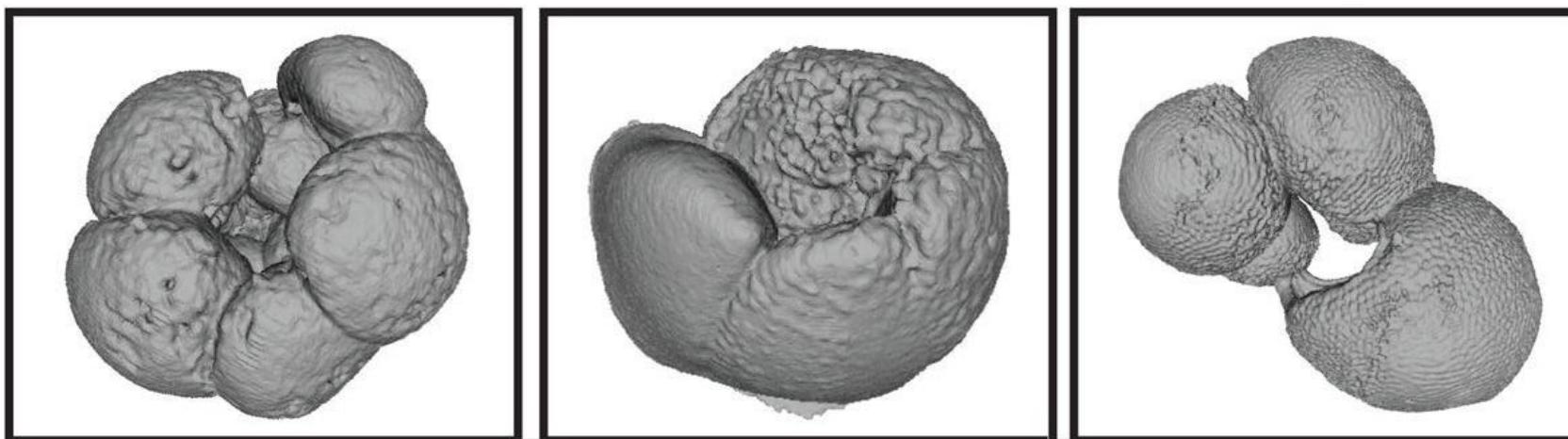
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Limitations of traditional landmarks

4) Cannot be used for “topology” changes

- i.e., differences reflecting missing features will not be quantified (Zelditch et al., 2004)
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Definition of ‘automated correspondence’

“biologically meaningful (possibly homologous) points are identified between pairs of digitized structures without human intervention except through manipulation of the algorithm parameters”

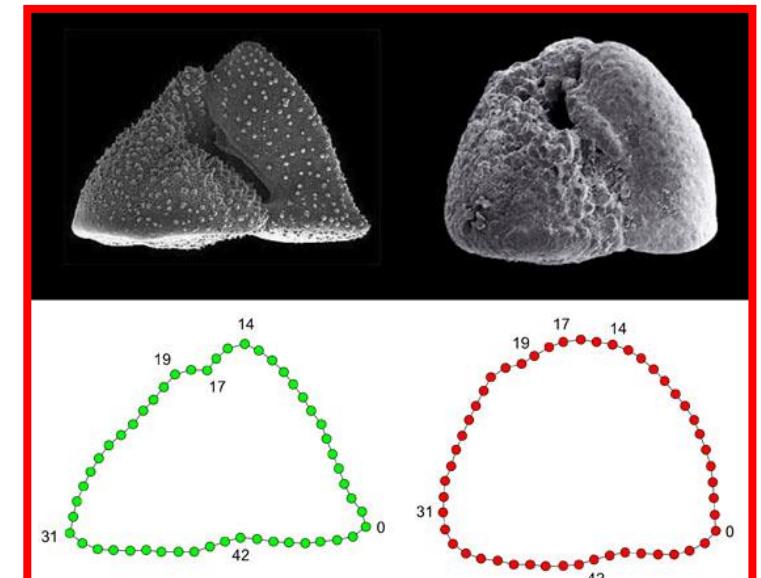
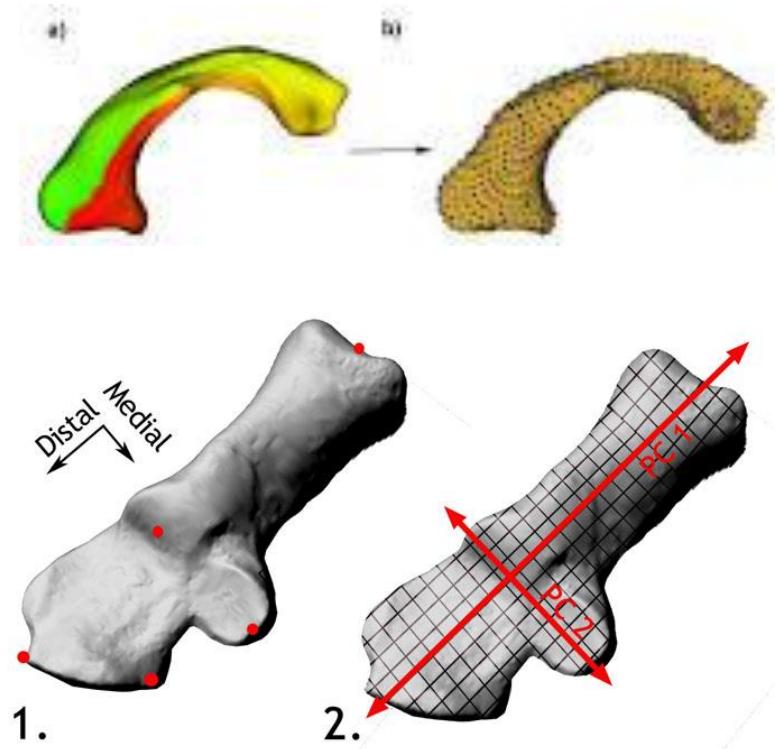
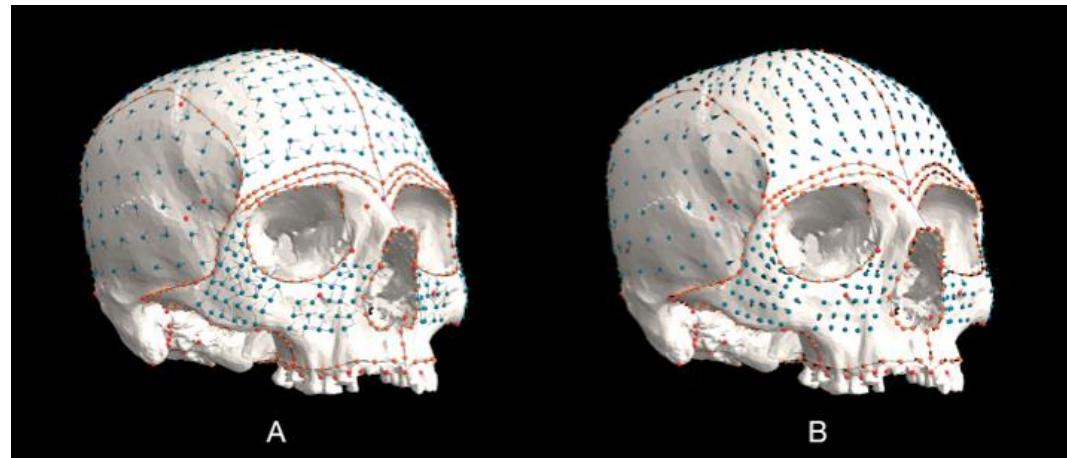
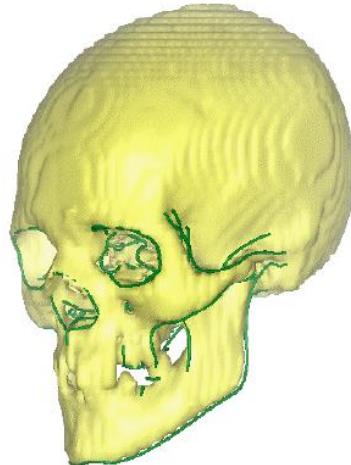
Initial Progress

Semi-automated methods

- Lohmann 1983, Weeks 1999, various papers in MacLeod 2007, Polly & MacLeod 2008, Sievwright et al. 2012, Mitteroecker & Gunz 2009

Automated methods restricted to conservative samples

- Thirion & Guordon 1996, Subsol et al. 2002, Styner et al. 2006, Paniagua et al. 2012



Automated approaches and their limitations thus far

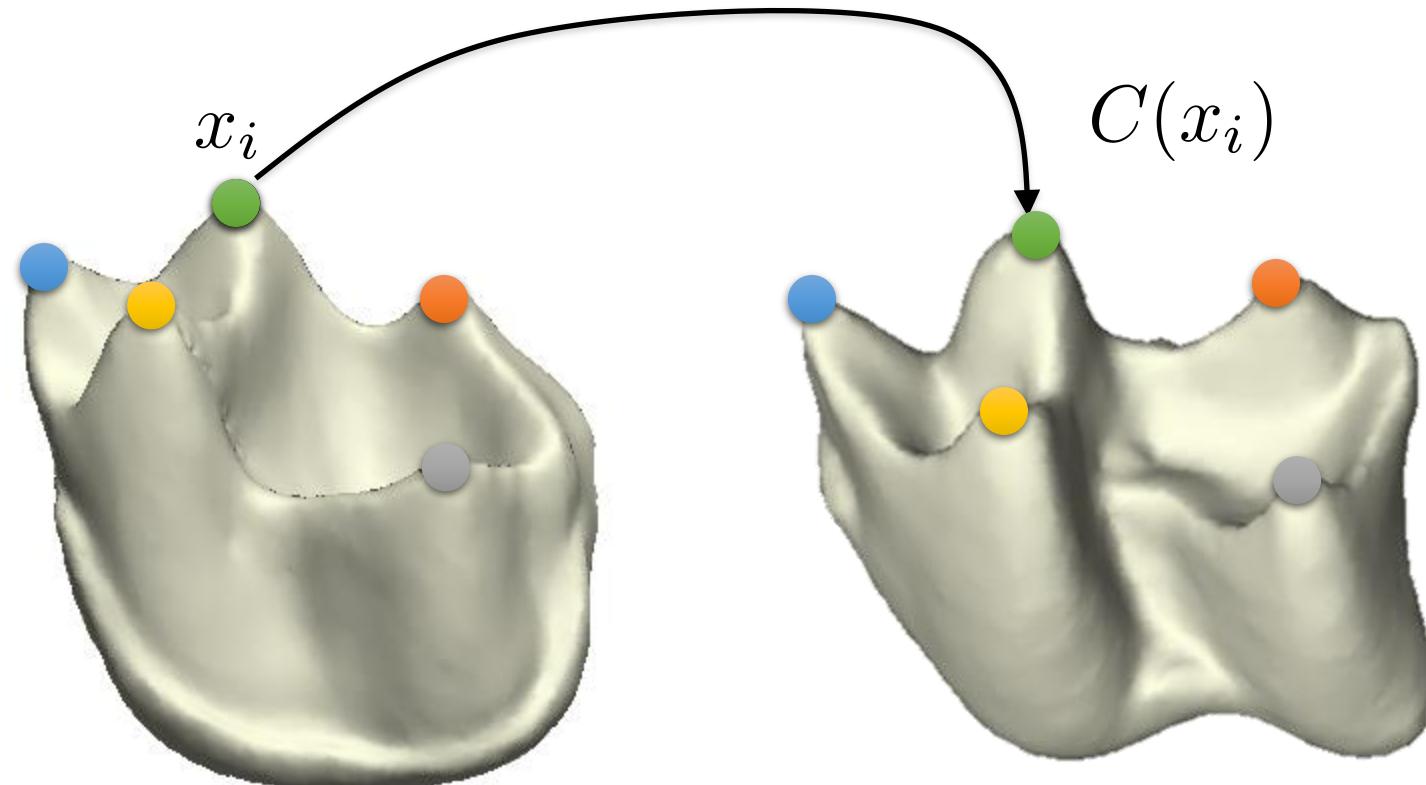
- Require an observer to supply an orientation or initial guess
 - For photography (to work from 2D images)
 - For choosing a orientation (Eigensurface of Polly & MacLeod, 2008)
 - Aligning “crest lines” (Thirion & Guordon, 1995; Subsol et al., 2002)
- Expect minimal variation
 - Clinical work on human-only samples (Styner et al. 2003)
 - Work with model animals (intraspecific variation)
- Computationally prohibitive
 - Biggest hurdle is finding correct initial alignment for diverse samples (e.g., Iterative Closest Points algorithm)

Solution (?)

- Identify ways to reduce # of likely candidate alignments and correspondences *a priori*
- Utilize Procrustes to find the ‘best’ among the candidates.



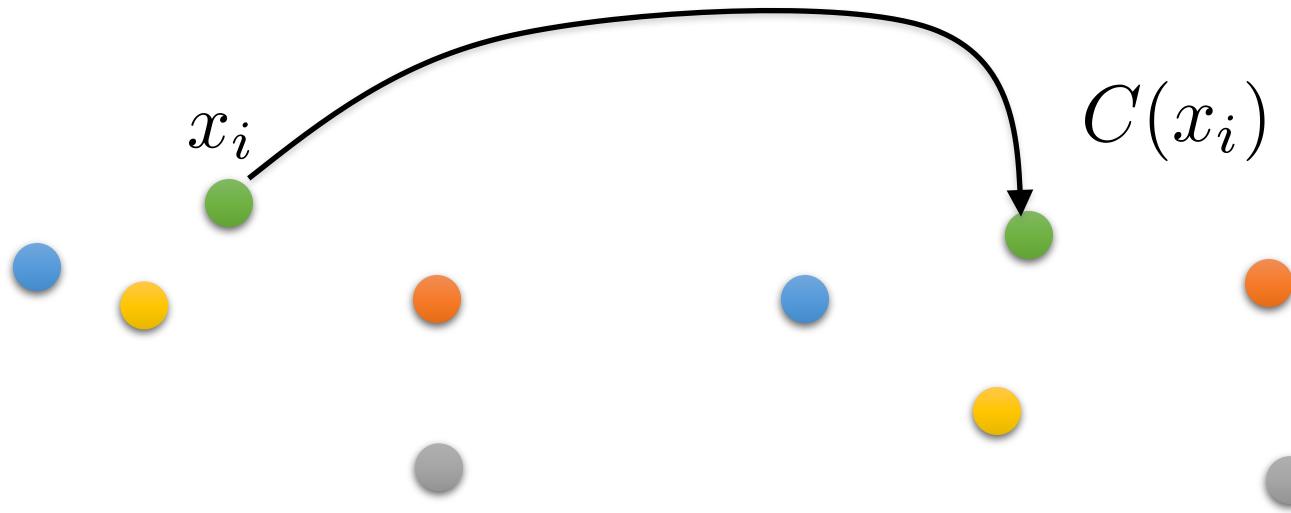
Standard Procrustes Distance



$C(x_i)$

“qualitatively determined”

Standard Procrustes Distance



$C(x_i)$ “qualitatively determined”

Find rigid motions (translation & rotation) that minimize sum distance

Modified Procrustes Distance

$C(x_i)$ is not specified *apriori*



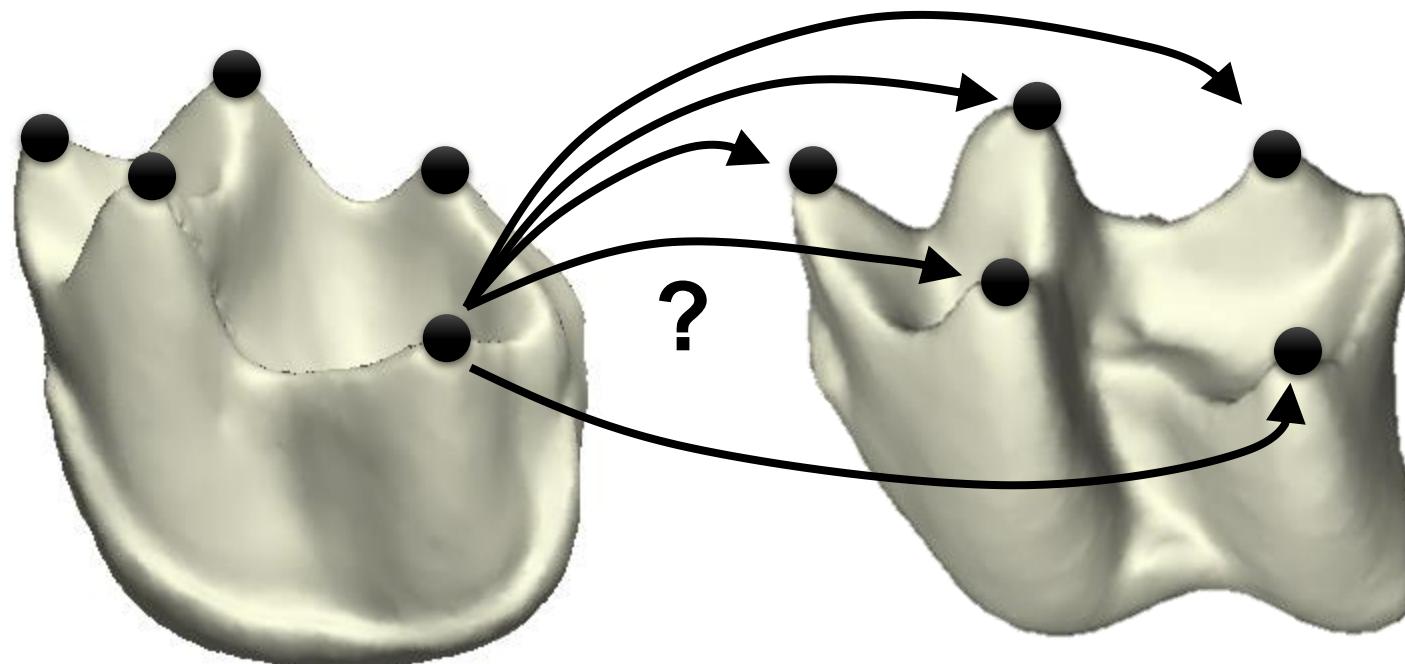
Find Correspondence map (C) that minimizes sum
distance, allowing any set of rigid motions

Modified Procrustes Distance

Find C with minimum Procrustes

5 points = 120 possibilities....

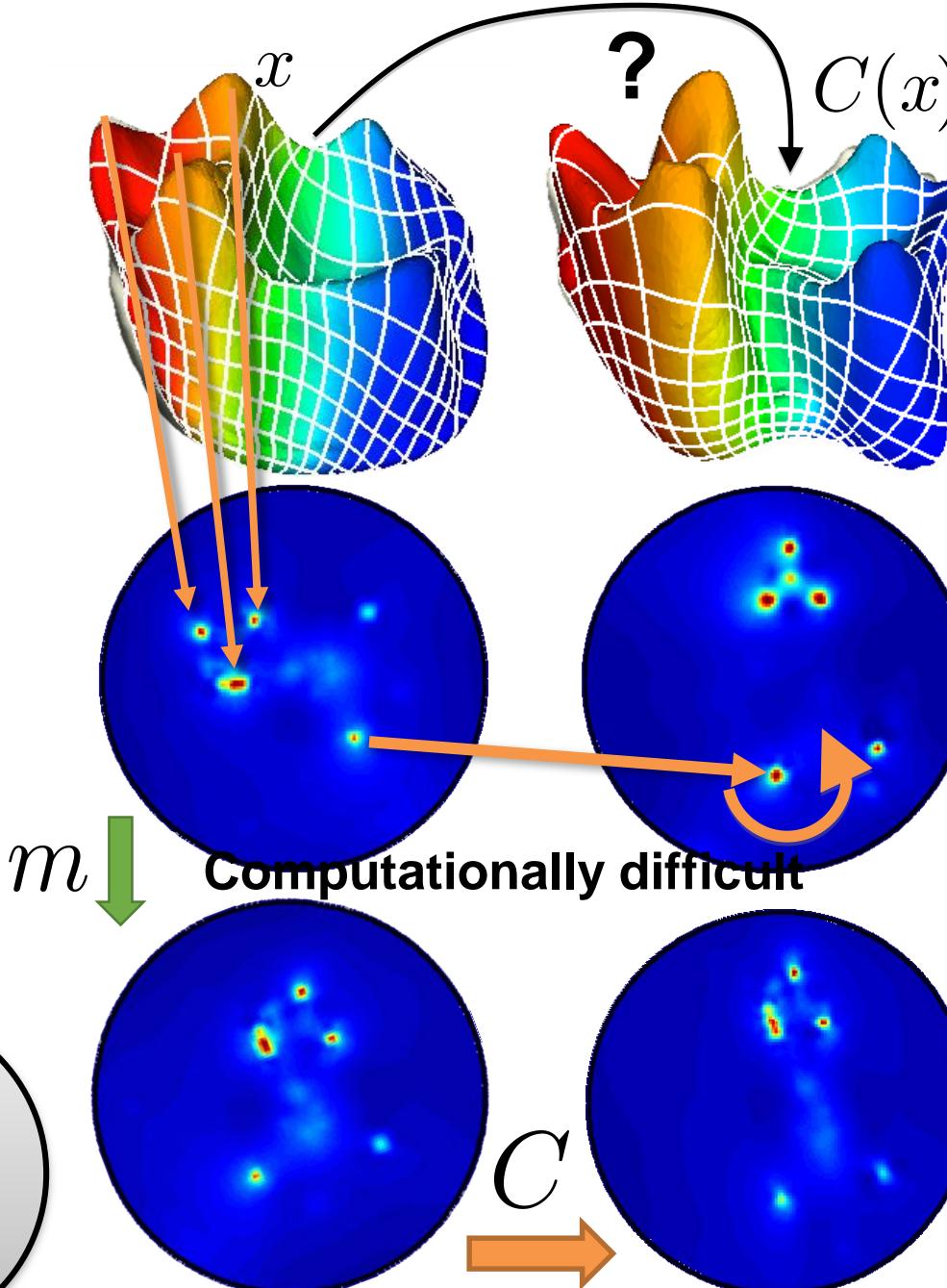
10 points = 3.6 million possibilities



Search area of
Correspondence
Maps...

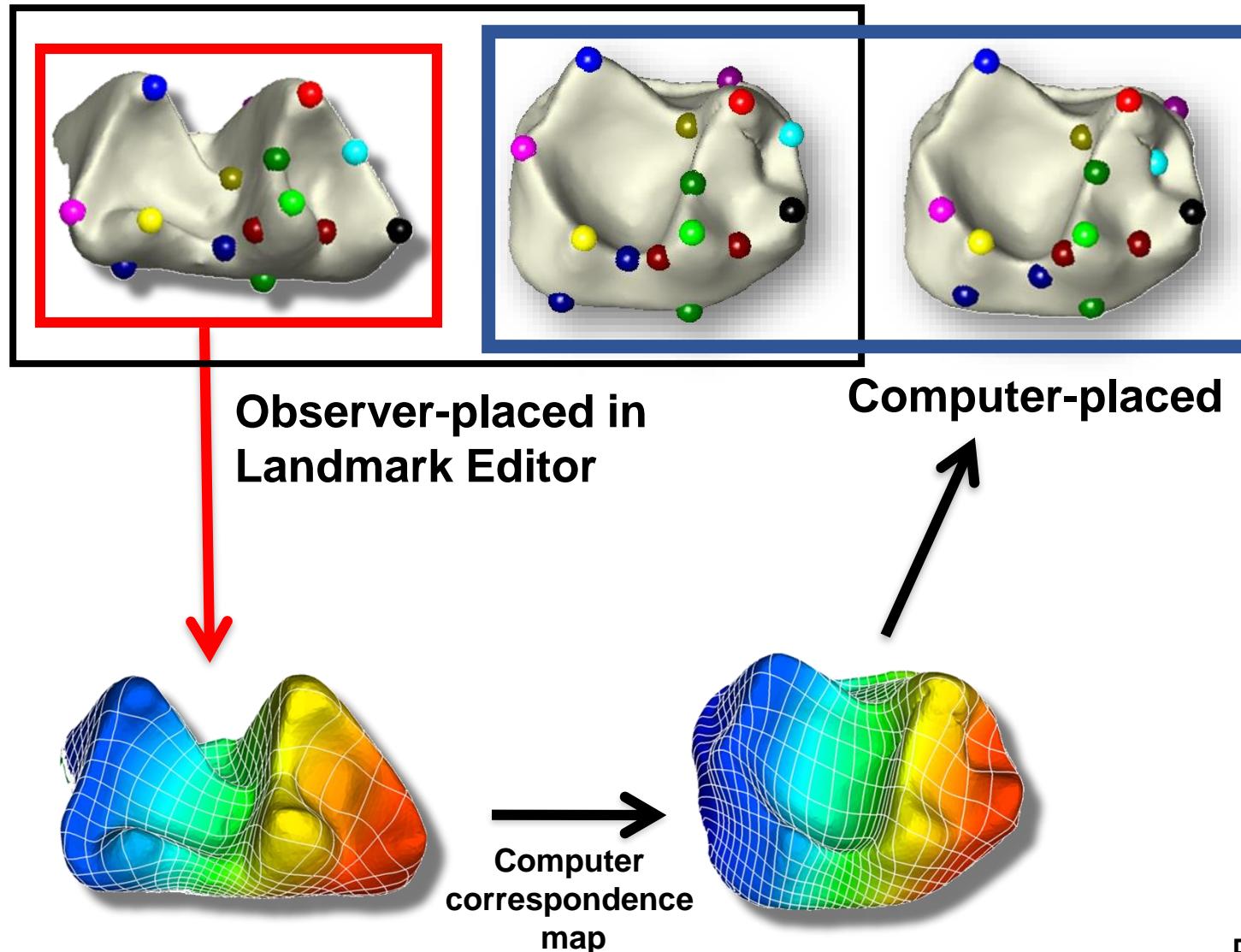
∞ Degrees of freedom

C
TPS
 m
Möbius
Maps
3 Degrees



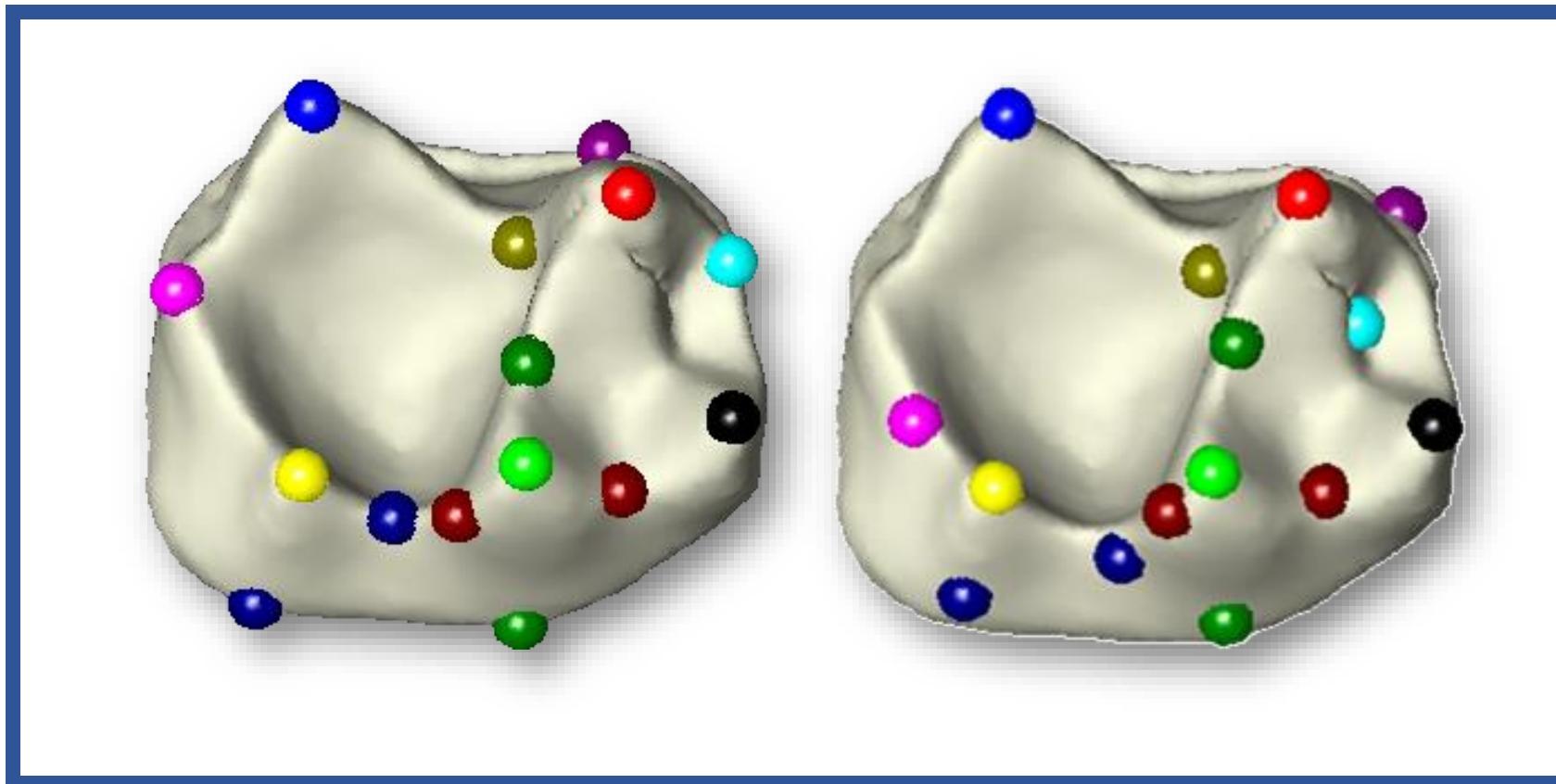
Results

Compare to Observer Landmarks



Results

Compare to Observer Landmarks



**Observer-placed
in
Landmark Editor**

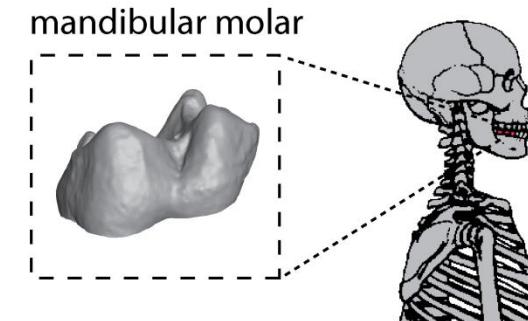
Computer-placed

CLASSIFICATION ANALYSIS

3 data sets (mainly primates)

116 mandibular 2nd molars

5 orders, 19 families, 35 genera



45 distal radii

1 order, 2 families, 4 genera

61 proximal first metatarsals (Mt1)

1 order, 9 families, 13 genera

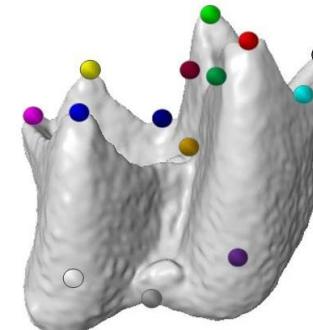
HUMAN correspondences

Same 3 data sets: Geometric landmarks applied

116 mandibular 2nd molars

5 orders, 19 families, 35 genera

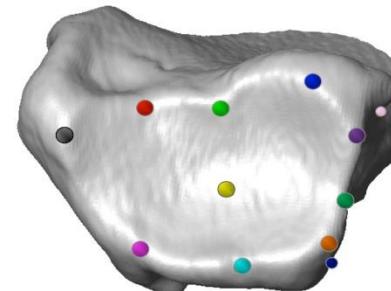
16 Landmarks



45 distal radii

1 order, 2 families, 4 genera

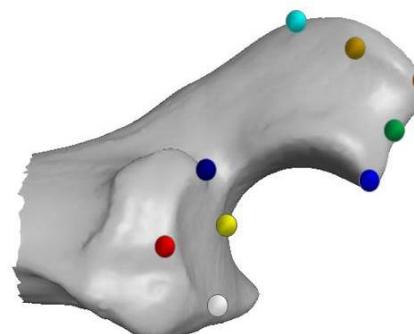
13 Landmarks



61 proximal Mt1

1 order, 9 families, 13 genera

11 Landmarks



Results

Classification success (mean % correct per genus)

Dataset	HUMAN correspondences	COMPUTER correspondences
Teeth 24 grps		
Radii 5 grps		
Mt1 13 grps		

Results

Classification success (mean % correct per genus)

Dataset	HUMAN correspondences	COMPUTER correspondences
Teeth 24 grps	90%	90%
Radii 5 grps		
Mt1 13 grps		

Results

Classification success (mean % correct per genus)

Dataset	HUMAN correspondences	COMPUTER correspondences
Teeth 24 grps	90%	90%
Radii 5 grps	83%	88%
Mt1 13 grps		

Results

Classification success (mean % correct per genus)

Dataset	HUMAN correspondences	COMPUTER correspondences
Teeth 24 grps	90%	90%
Radii 5 grps	83%	88%
Mt1 13 grps	76%	82%

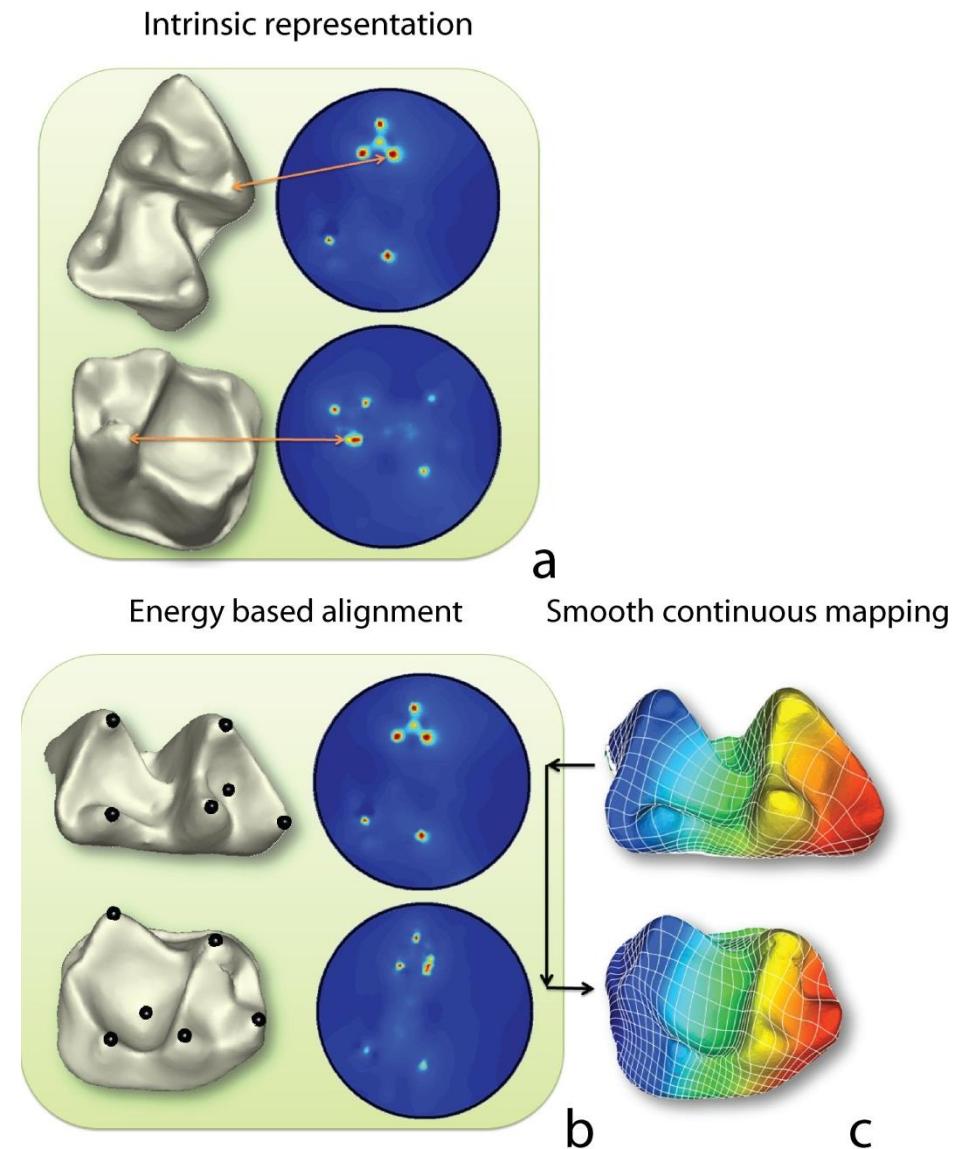
Initial Progress

First automated correspondence algorithm in 3D (Boyer et al. 2011)

- Tested on three samples of surface models (teeth, radii, metatarsals)
- Compared to traditional landmark data sets on same samples

Results

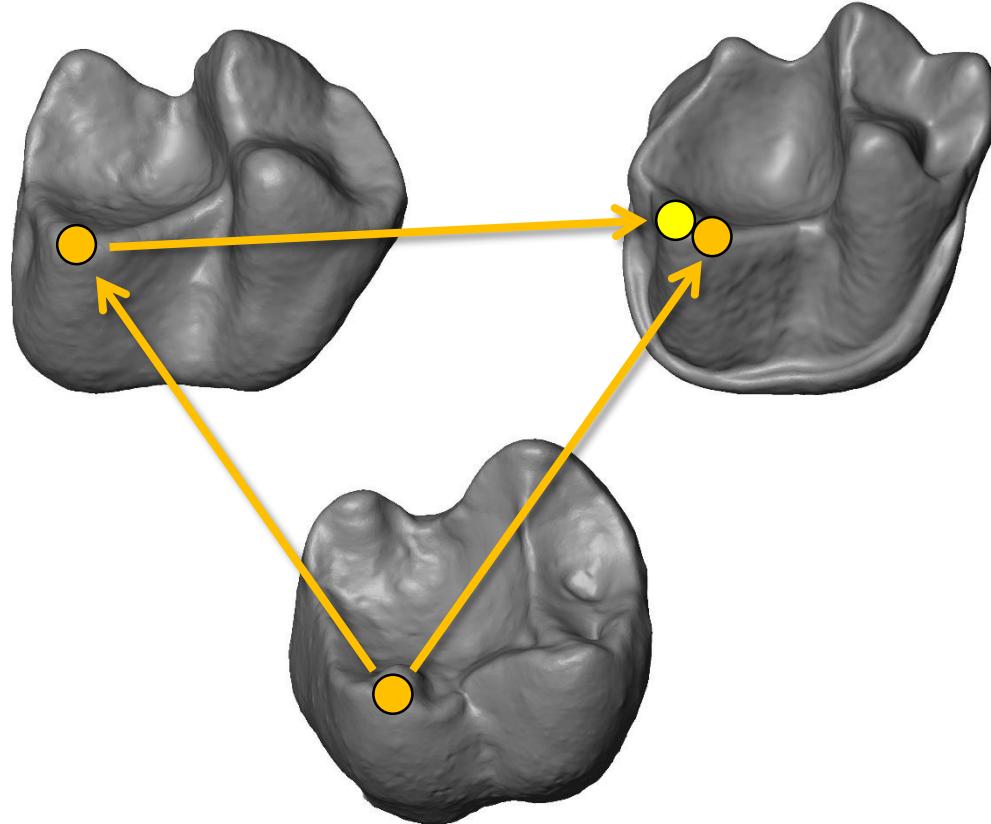
- Produced plausible correspondence maps
- Automatically determined distances correlated as strongly with taxonomic differences as distances based on manually-collected data.



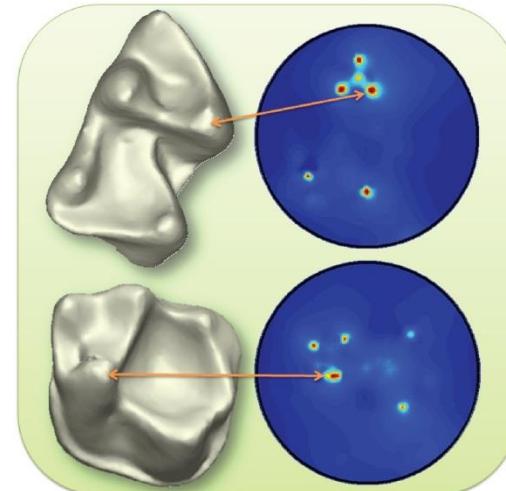
Initial Progress

Limitations

- Difficult to work with Matlab code
- Correspondence determinations non-transitive
- Poor alignment with most dissimilar shapes



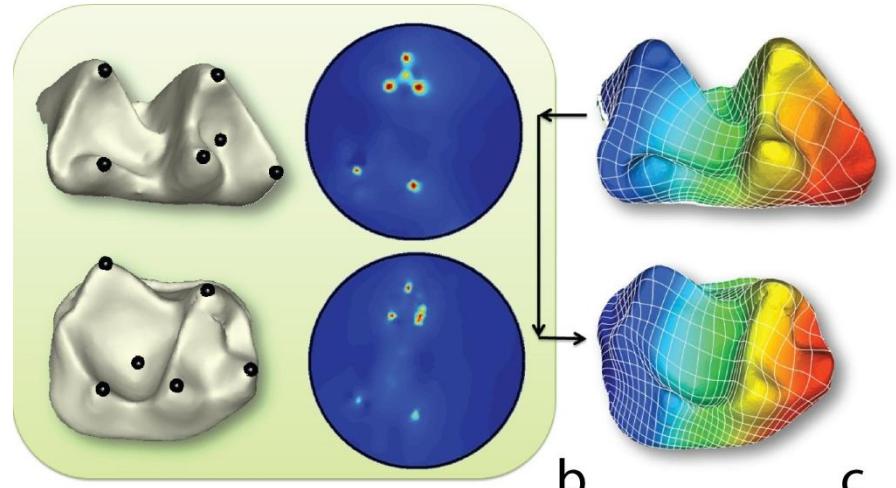
Intrinsic representation



Energy based alignment

a

Smooth continuous mapping



b

c

Auto3dgm: Concepts & Logistics

- Similar objects are easy to align automatically
- Use a graded series of similar objects to align dissimilar endmembers
- Exists as R, matlab, and now Python / Slicer routines.
- Transitive correspondences
- Output includes a landmark file that can be analyzed with standard 3d geometric morphometric software (including Morphologika, MorphoJ and SlicerMorph)
- Can be used for alignment of 3D models
- Provides a way to compare magnitude of variation between two samples

Auto3dgm: Publications

Methodological/validation

- Boyer et al. (2015): <https://onlinelibrary.wiley.com/doi/full/10.1002/ar.23084>
- Boyer et al. (2016): <https://onlinelibrary.wiley.com/doi/abs/10.1002/ar.23202>
- Gonzalez et al. (2016): <https://onlinelibrary.wiley.com/doi/abs/10.1002/ajpa.22934>
- Gao et al. (2017): <https://onlinelibrary.wiley.com/doi/abs/10.1002/ar.23700>
- Gao et al. (2018): <https://arxiv.org/pdf/1807.11887.pdf>

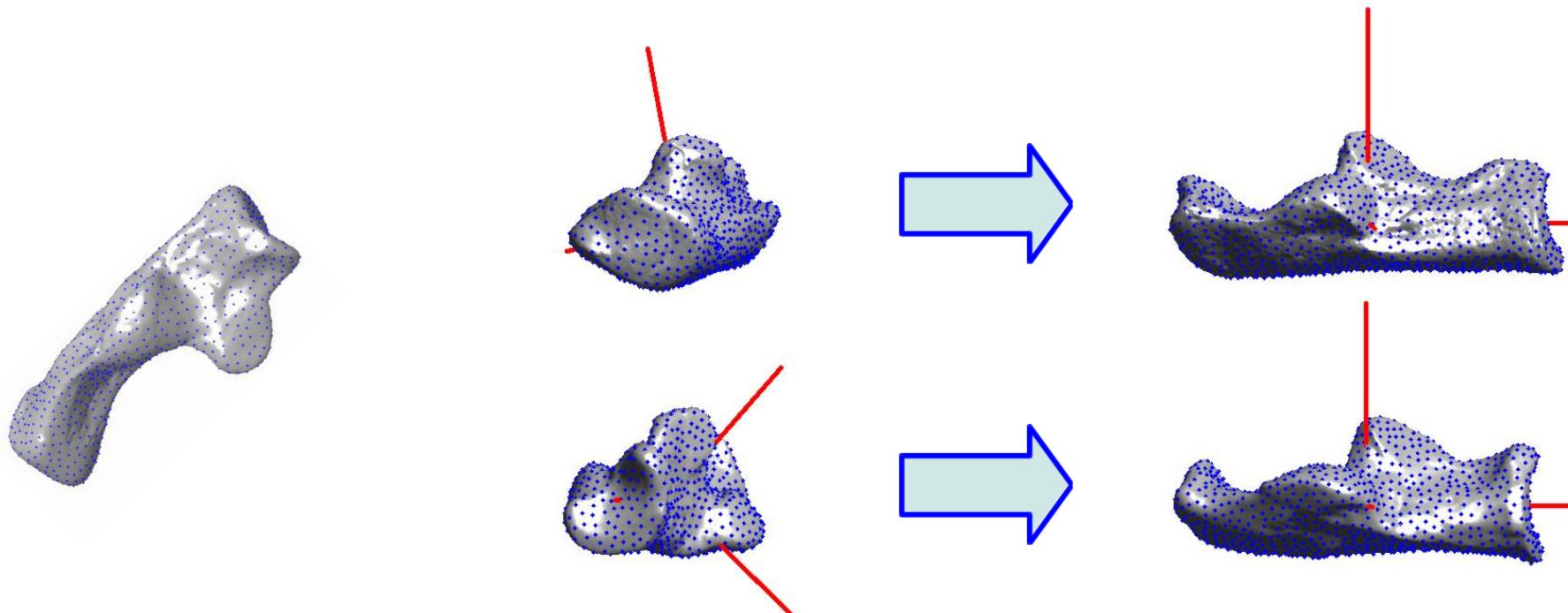
Applications (e.g.):

- Turner et al. (2014): <https://doi.org/10.1093/imaiai/iau011>
- Sieffert et al. (2015): <https://peerj.com/articles/1036/>
- Hsiang et al. (2016): <http://rstb.royalsocietypublishing.org/content/371/1691/20150227>
- Gingerich (2016): <https://link.springer.com/article/10.1007/s12542-017-0362-8>
- Boyer et al. (2017): <https://www.sciencedirect.com/science/article/pii/S0047248417301021>
- Vitek et al. (2017): <https://onlinelibrary.wiley.com/doi/abs/10.1002/ece3.3058>
- Renaud et al. (2017): <https://www.sciencedirect.com/science/article/pii/S0003996917301383?via%3Dihub>
- Renaud et al. (2018): <https://link.springer.com/article/10.1007/s11692-018-9459-6>
- Boyer et al. (2018): <https://www.sciencedirect.com/science/article/pii/S0047248417305134>
- Gunnell et al. (2018): <https://www.nature.com/articles/s41467-018-05648-w>
- Wang et al. (2019): <https://www.biorxiv.org/content/10.1101/701391v1>

Steps to the method

Processing and initial alignment

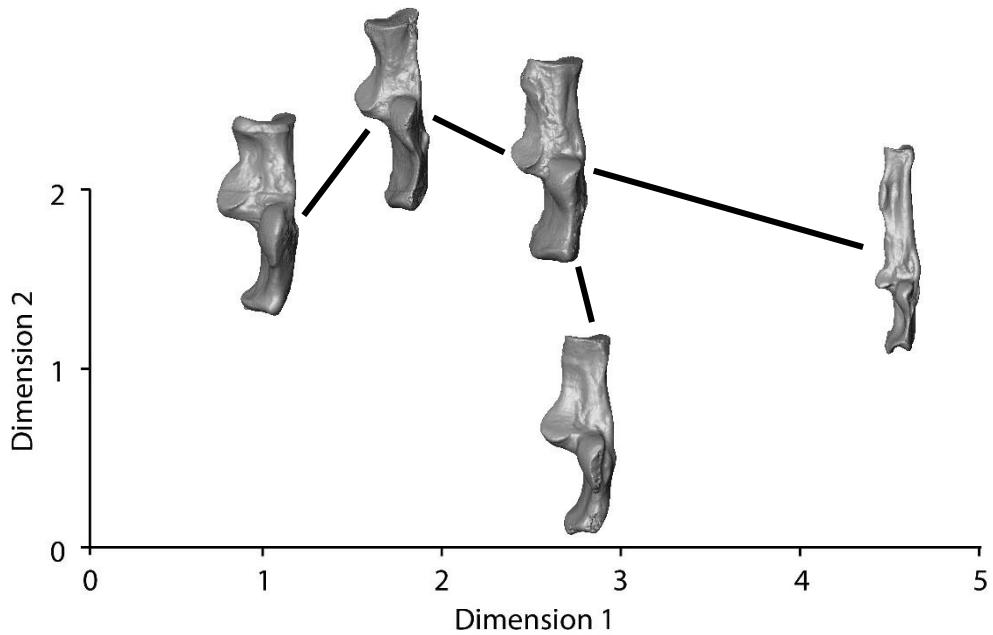
- Re-sample surface + size-standardize point cloud (Eldar et al. 1997)
- Compute principle axes with PCA
- Begin “alignment search”
 - Principle axes (8 possibilities)
 - Iterative closest points: Compute euclidean motions that minimize procrustes distance (PCD) (Besl & McKay 1992)



Steps to the method

Alignment refinement

- Compute Procrustes for all pairs
- Determine minimum spanning tree (MST)
- Propagate correspondences through MST for transitivity



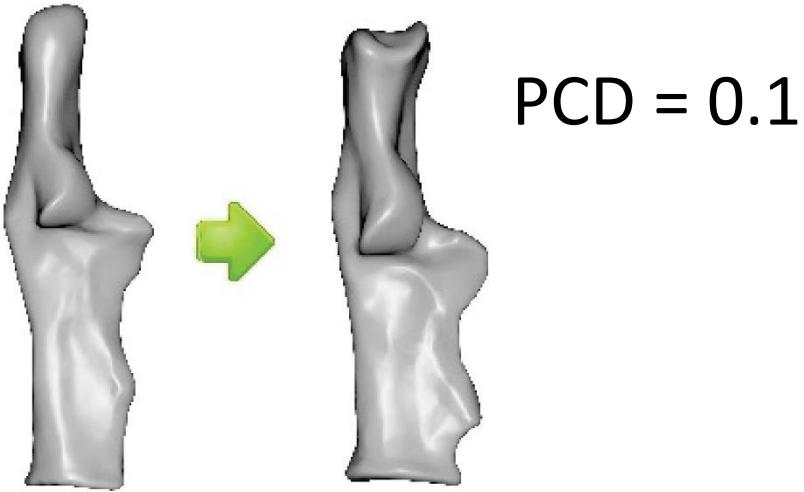
PCD matrix

	0	0.2	0.3	0.2	0.6
	0	0.2	0.1	0.5	
	0	0.3	0.6		
	0	0.4			
	0				

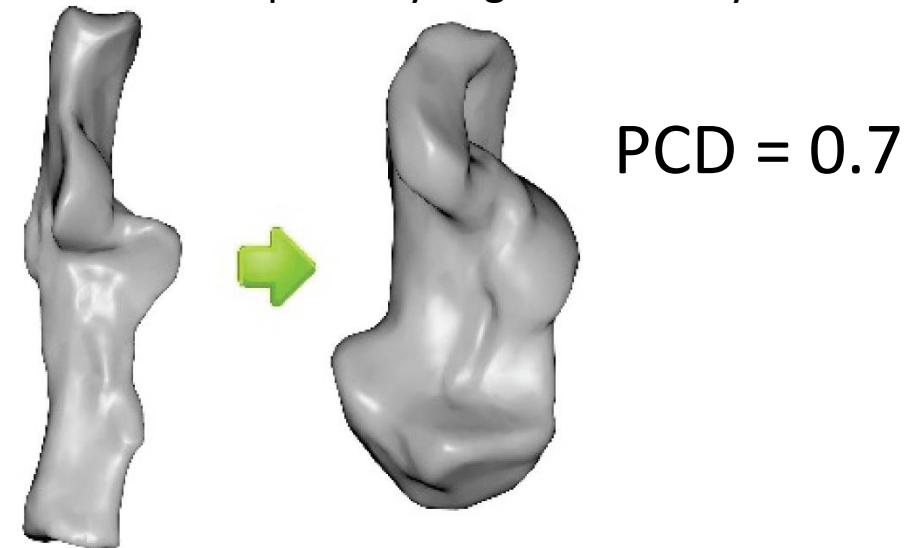
The table represents the Procrustes Distance (PCD) matrix for the five bone shapes. The diagonal elements are 0. The off-diagonal elements represent the Procrustes distances between pairs of bones. The values are: (0,1): 0, (0,2): 0.2, (0,3): 0.3, (0,4): 0.2, (0,5): 0.6; (1,2): 0, (1,3): 0.2, (1,4): 0.1, (1,5): 0.5; (2,3): 0, (2,4): 0.3, (2,5): 0.6; (3,4): 0, (3,5): 0.4; (4,5): 0.

Purpose of MST & Propagation

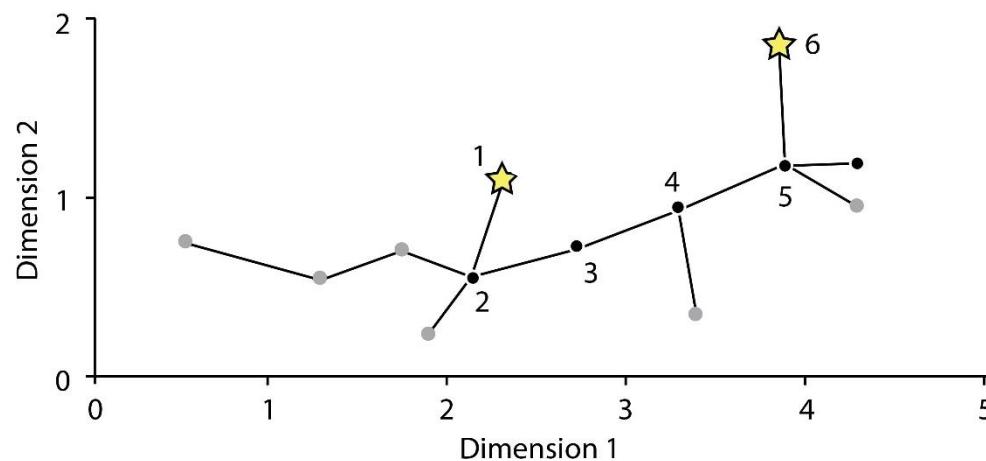
Similar shapes align well



Dissimilar shapes may align incorrectly

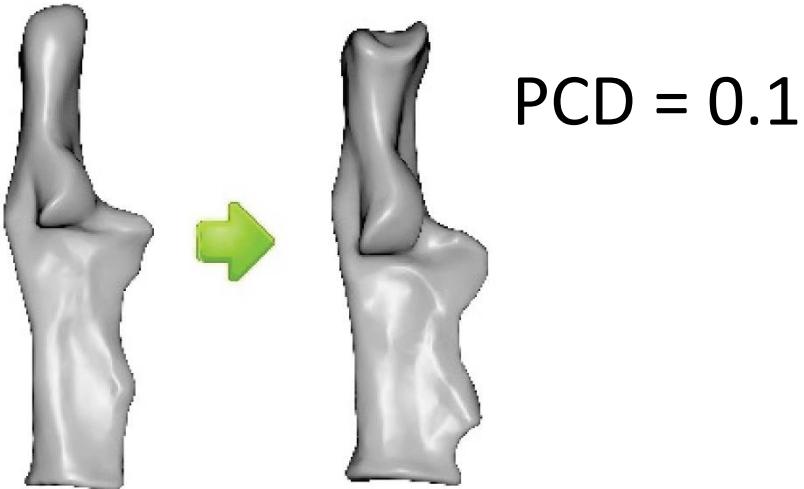


All Procrustes distances used to construct initial minimum spanning tree

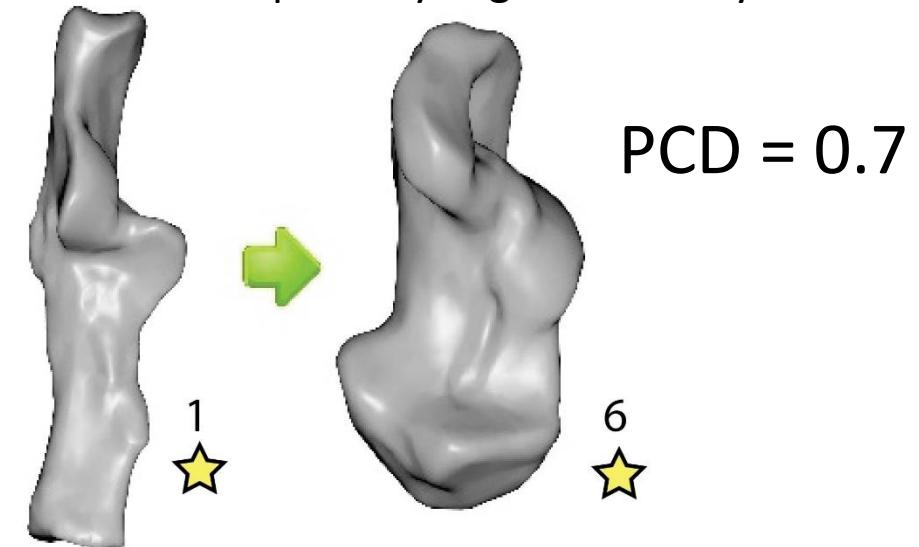


Purpose of MST & Propagation

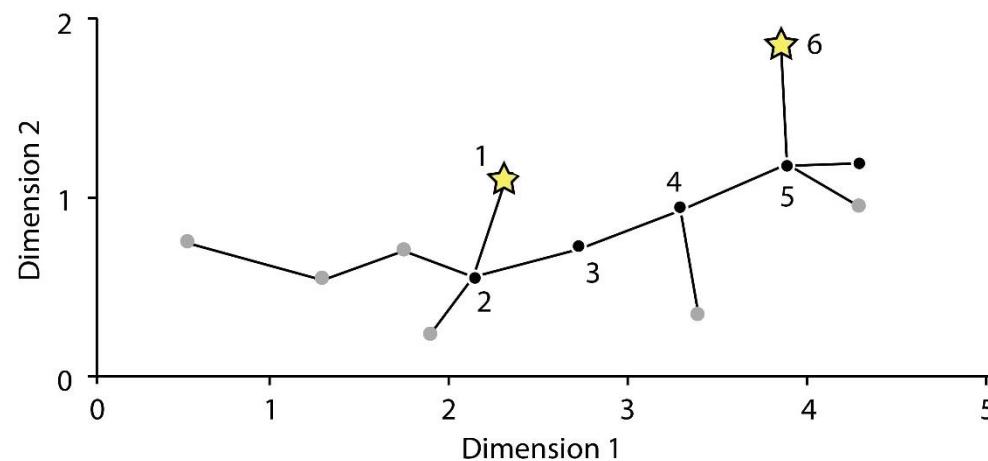
Similar shapes align well



Dissimilar shapes may align incorrectly

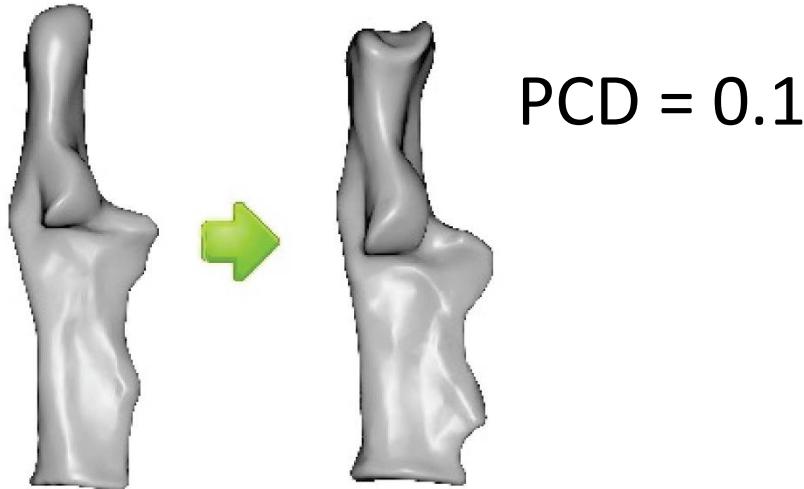


Incorrect alignments typically have high PCD and won't be in the MST

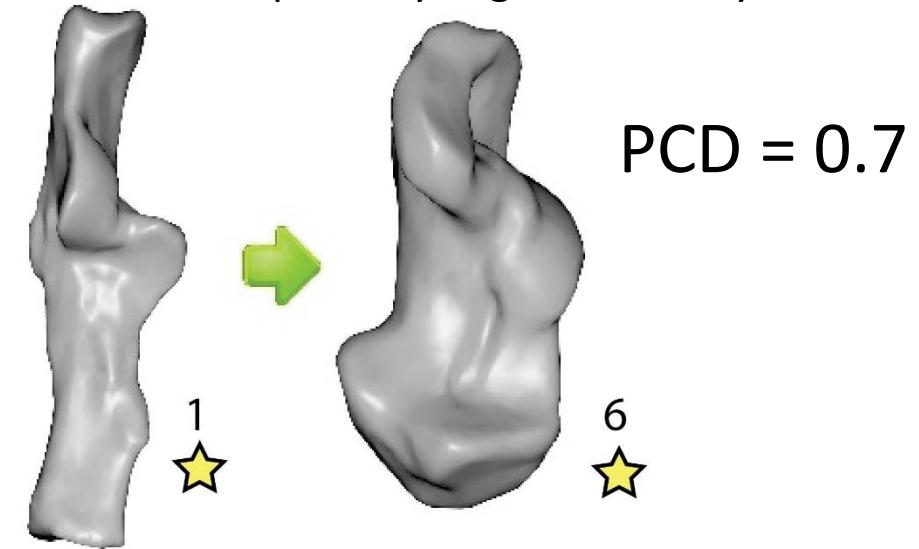


Purpose of MST & Propagation

Similar shapes align well



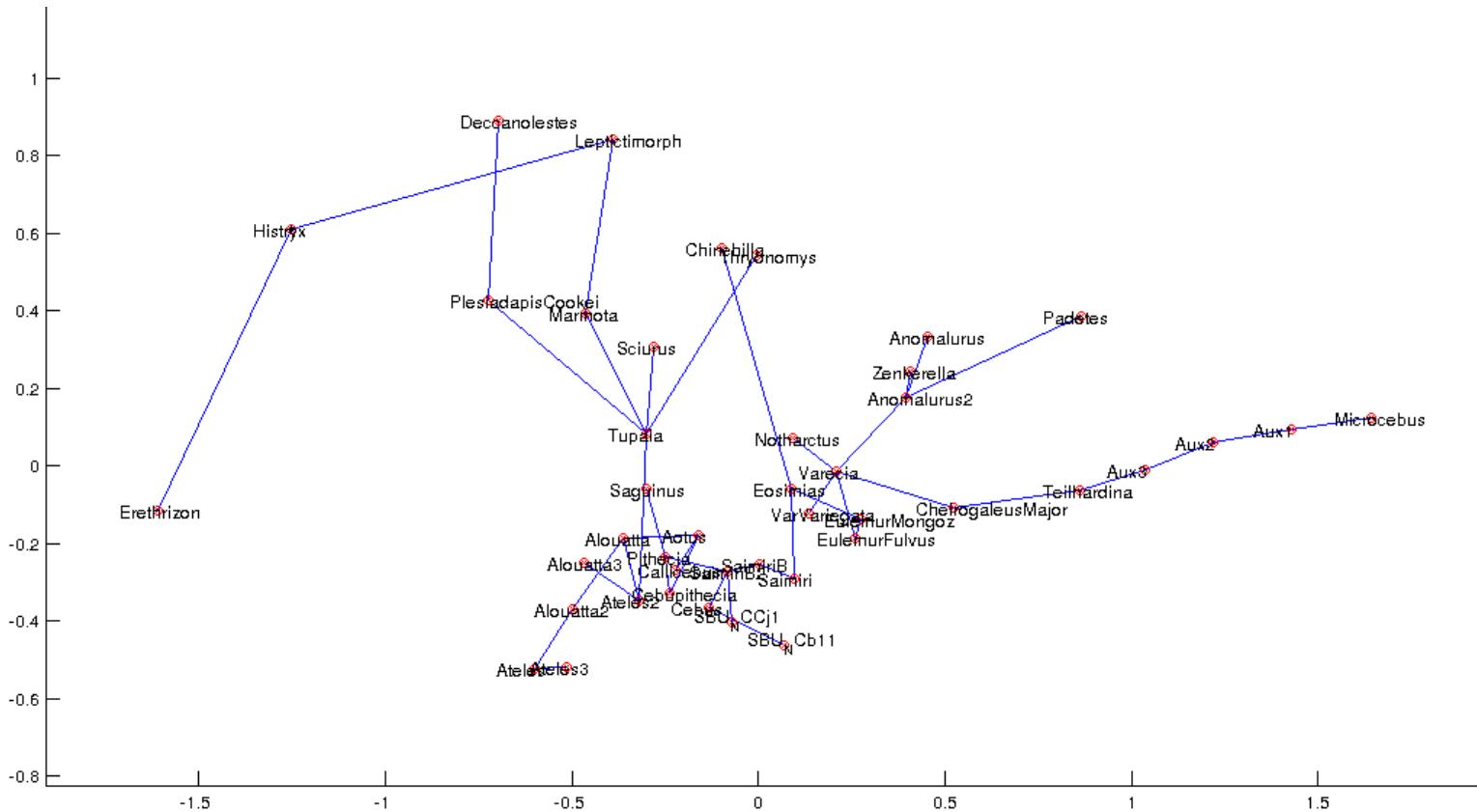
Dissimilar shapes may align incorrectly



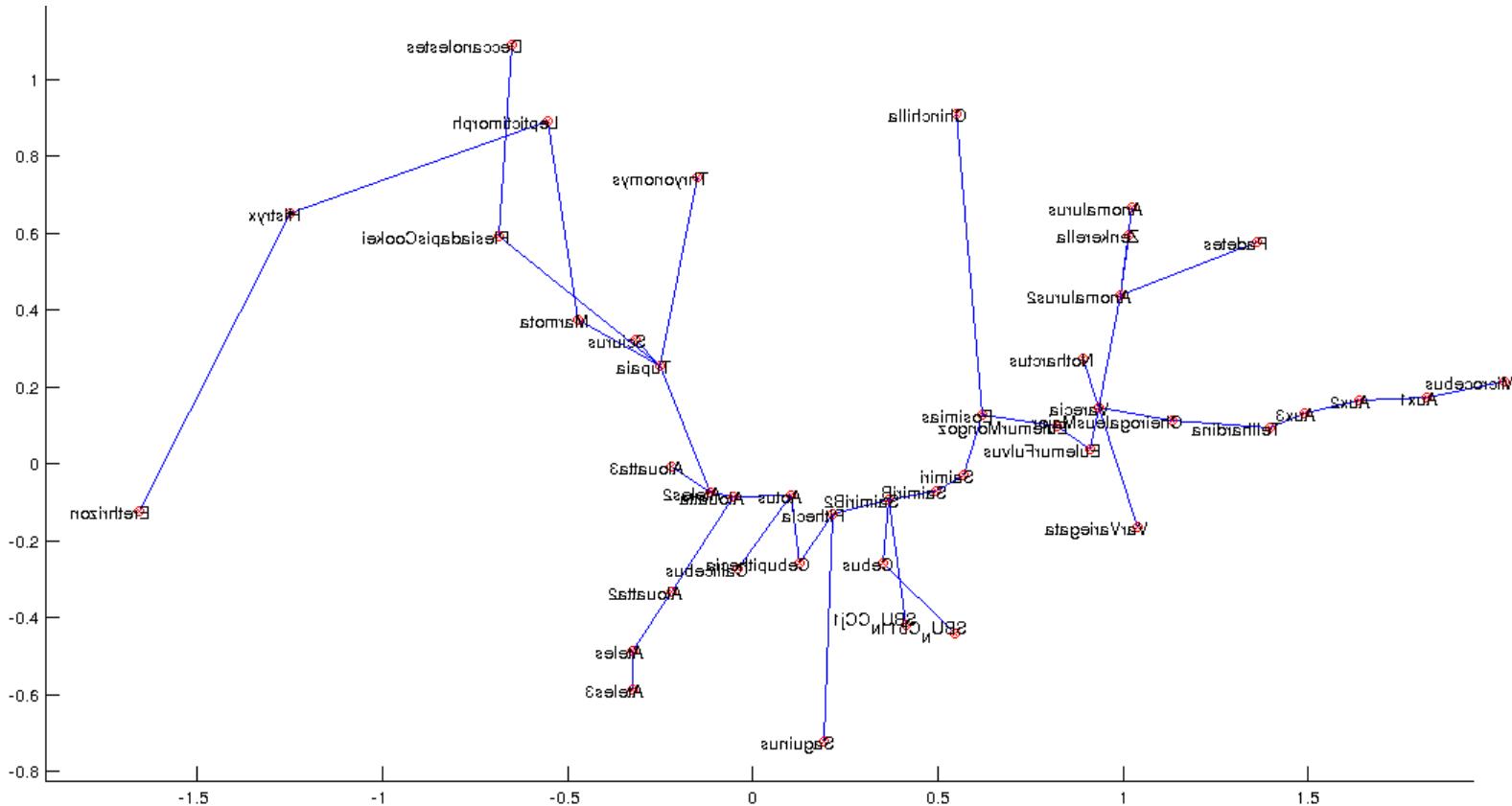
The MST path can be used to find correct alignments, and recompute distances



MST w initial correspondences

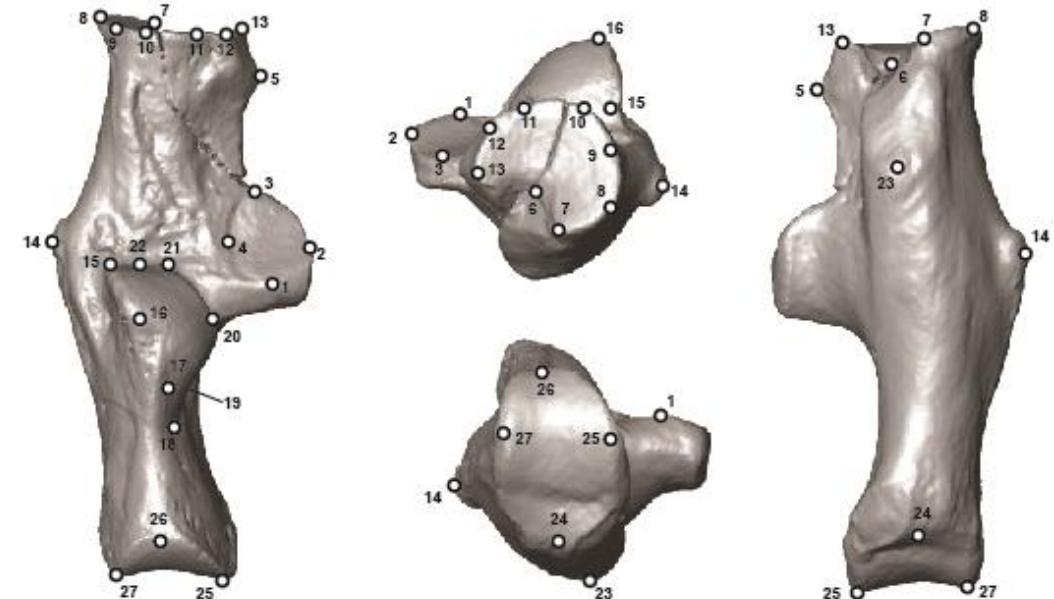


MST w transitive correspondences



Comparison to researcher-based data set

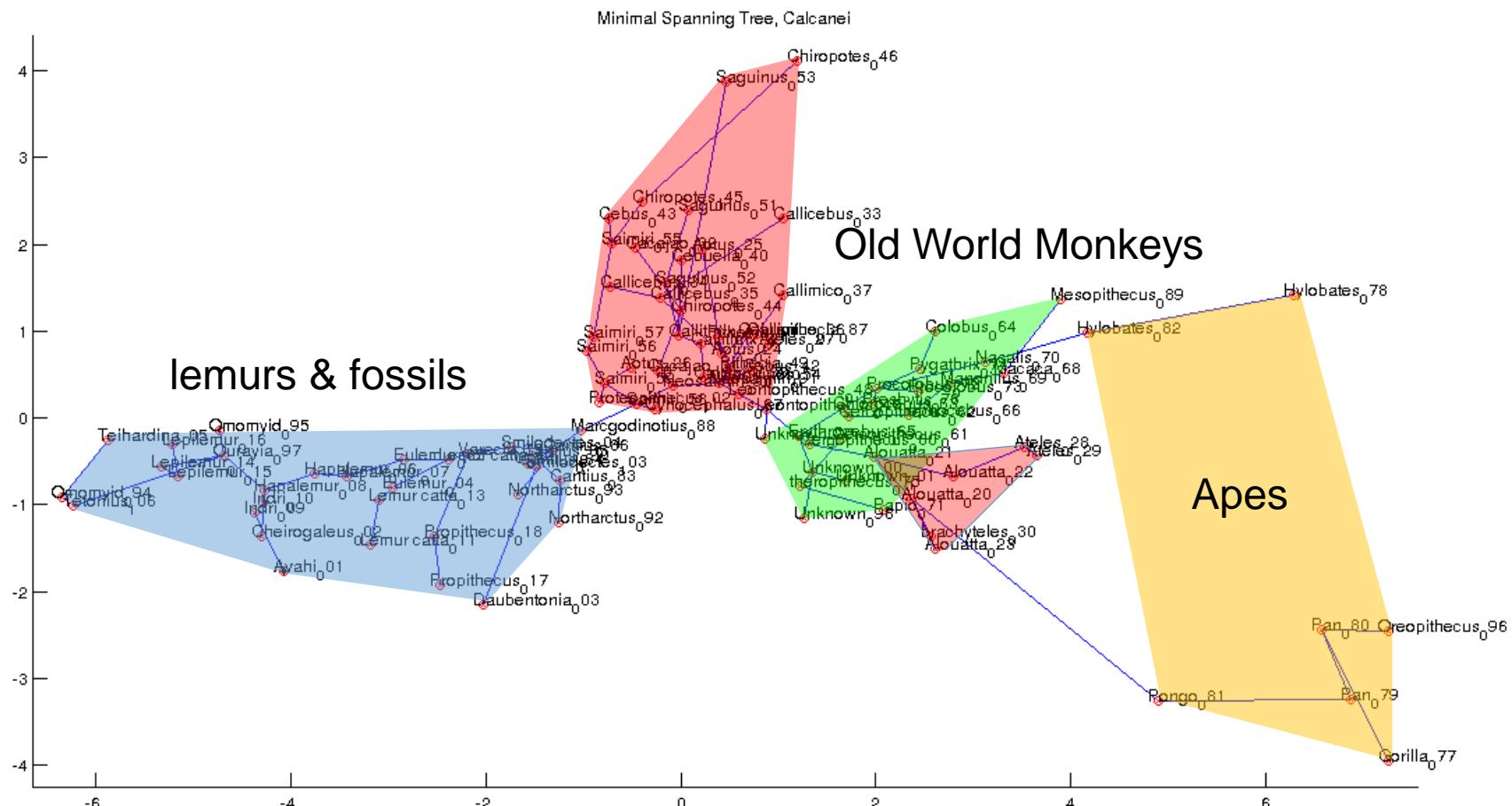
- Sample - 106 calcanei
- Data points
 - Observer (27 landmarks)
 - Algorithm (1,024 points)
- Software
 - *Morphologika2.5*
- Both datasets analyzed identically



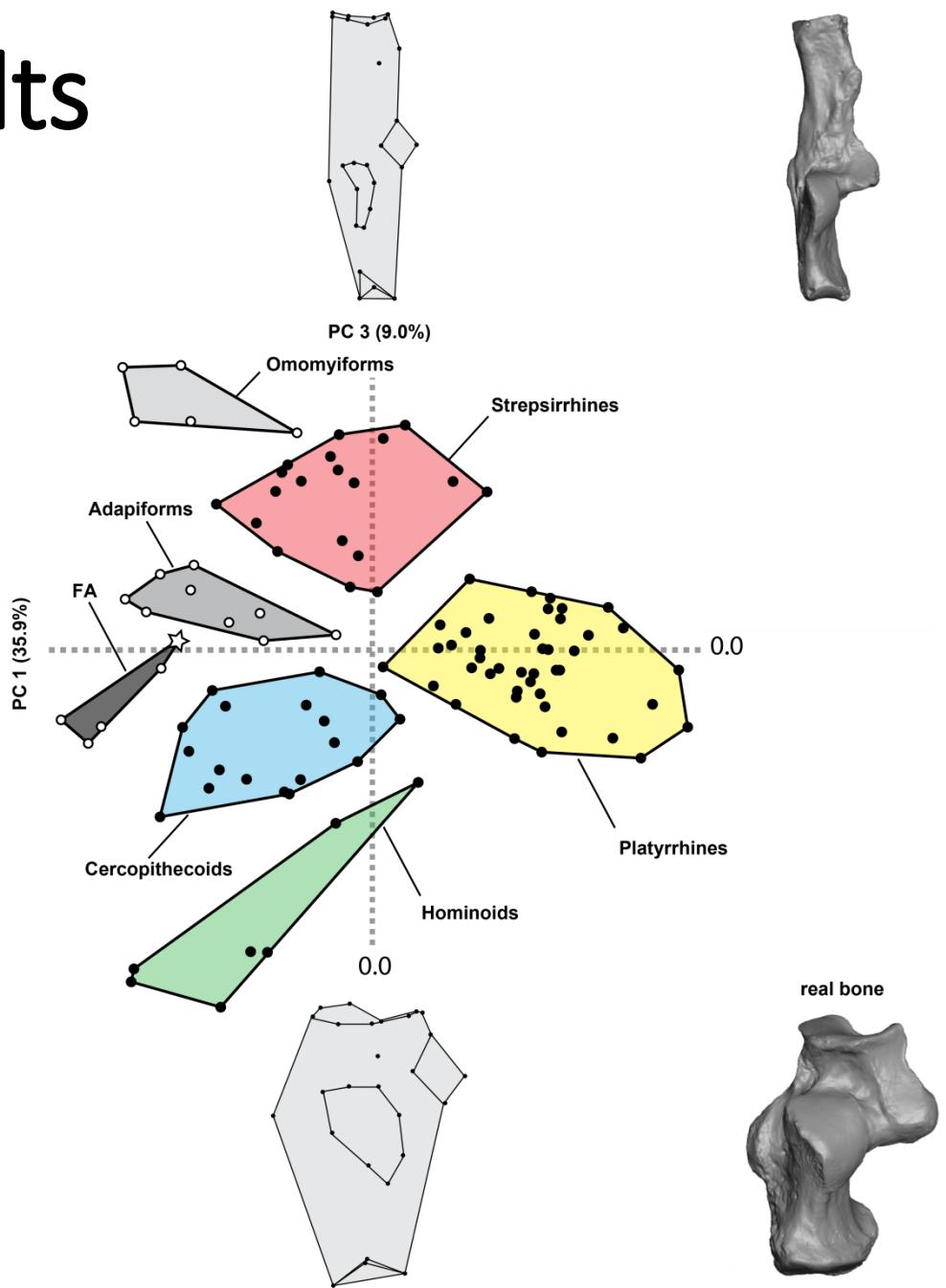
From Gladman et al. (2013)

Results

South American monkeys

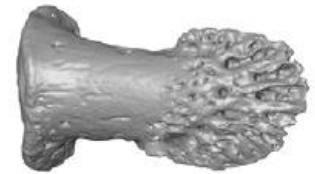
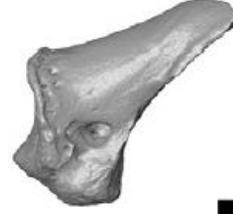


Results



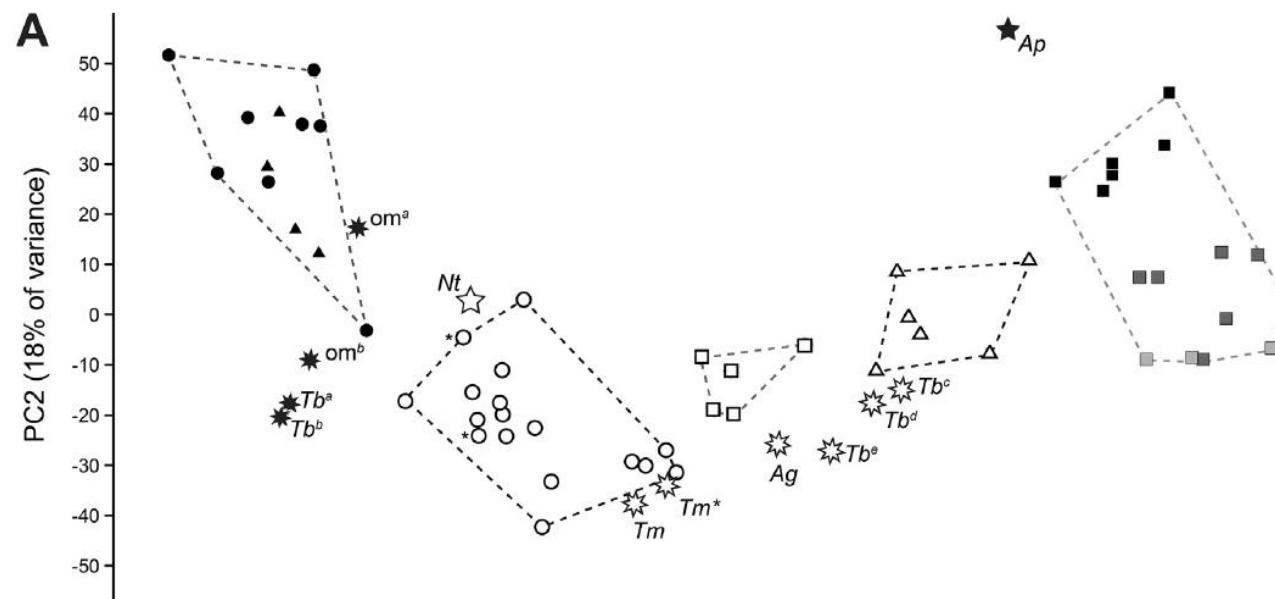
Difficult example

claws

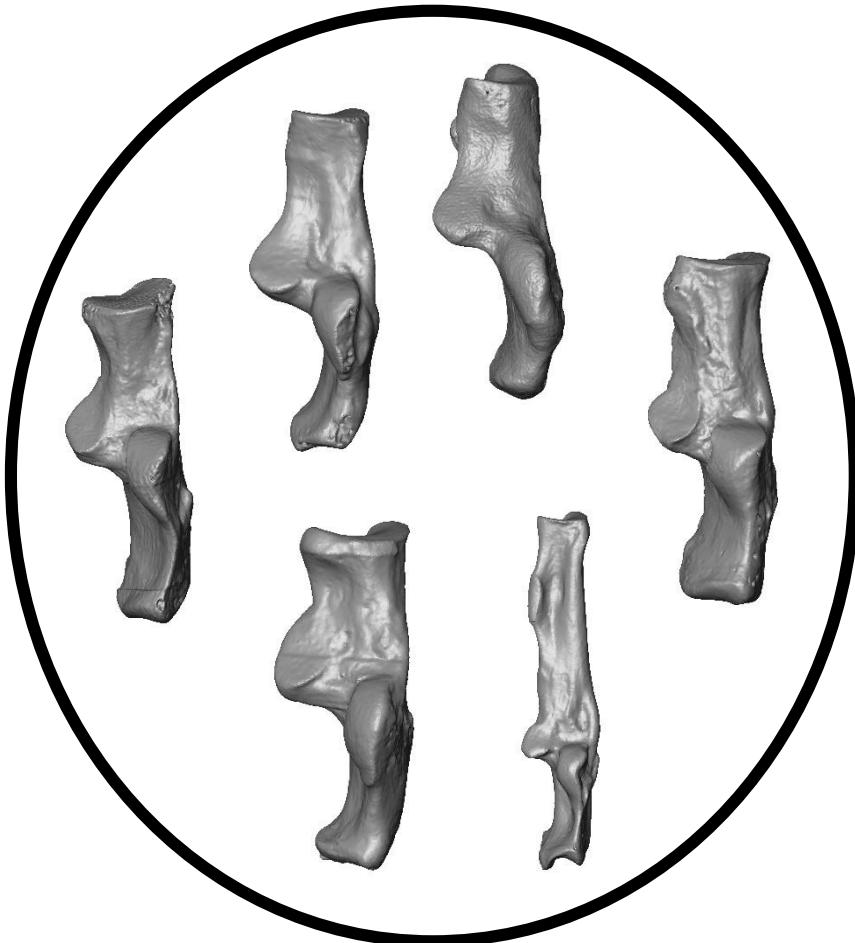


nails

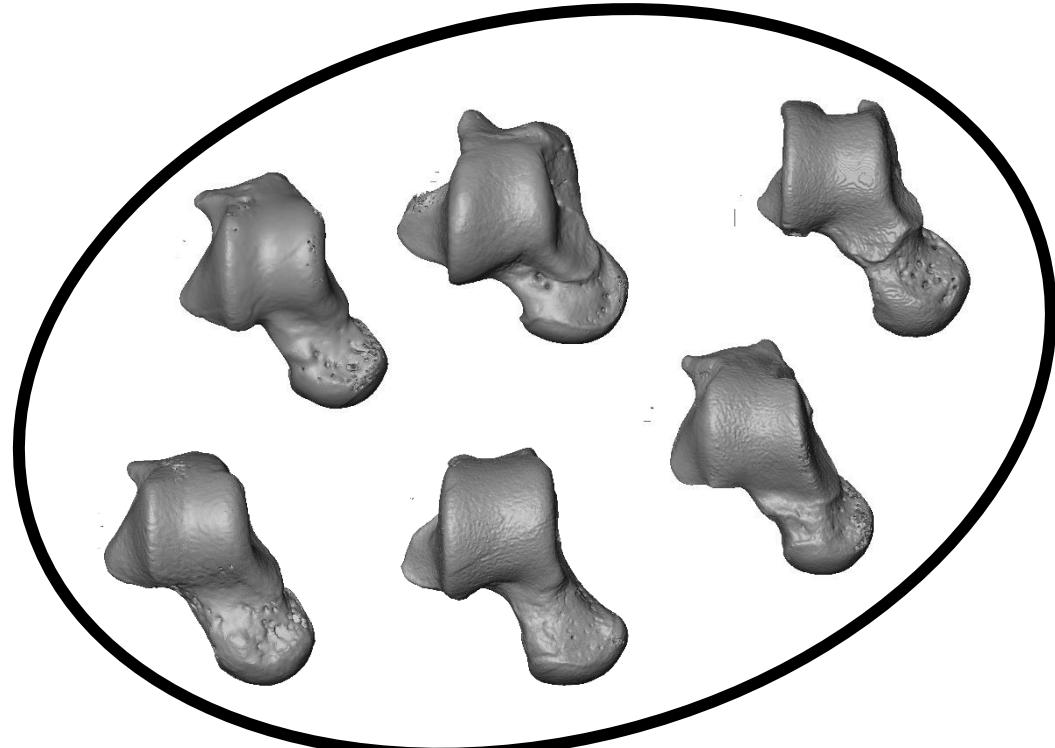
A



Comparison between bones

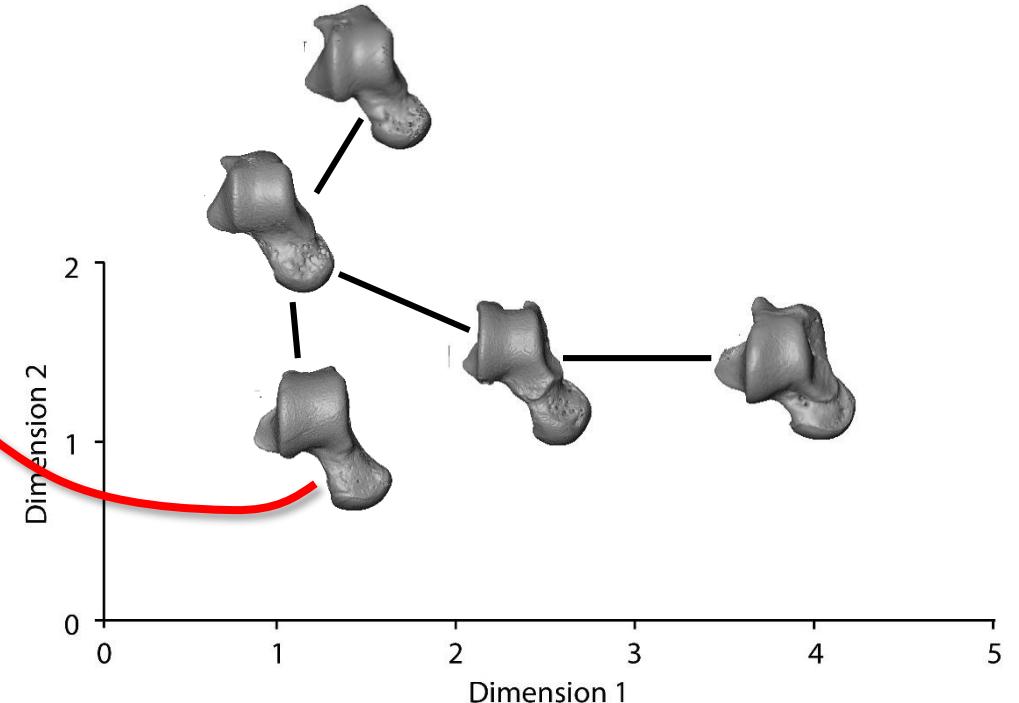
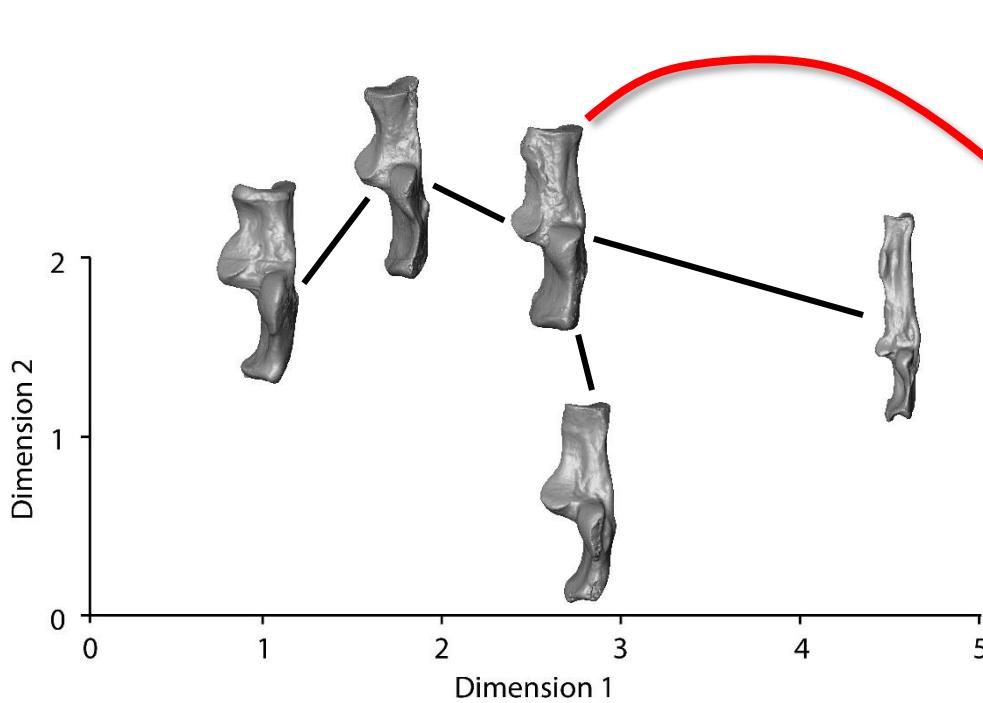


versus



Steps to the method

- Use standard number of points in each sample
- Analyze each bone type separately
- Compute Procrustes minimum distance for all pairs astragali+calcanei
- Link minimum spanning trees using pair with smallest PCD



Steps to the method

Yields global landmark dataset that applies to both bone types

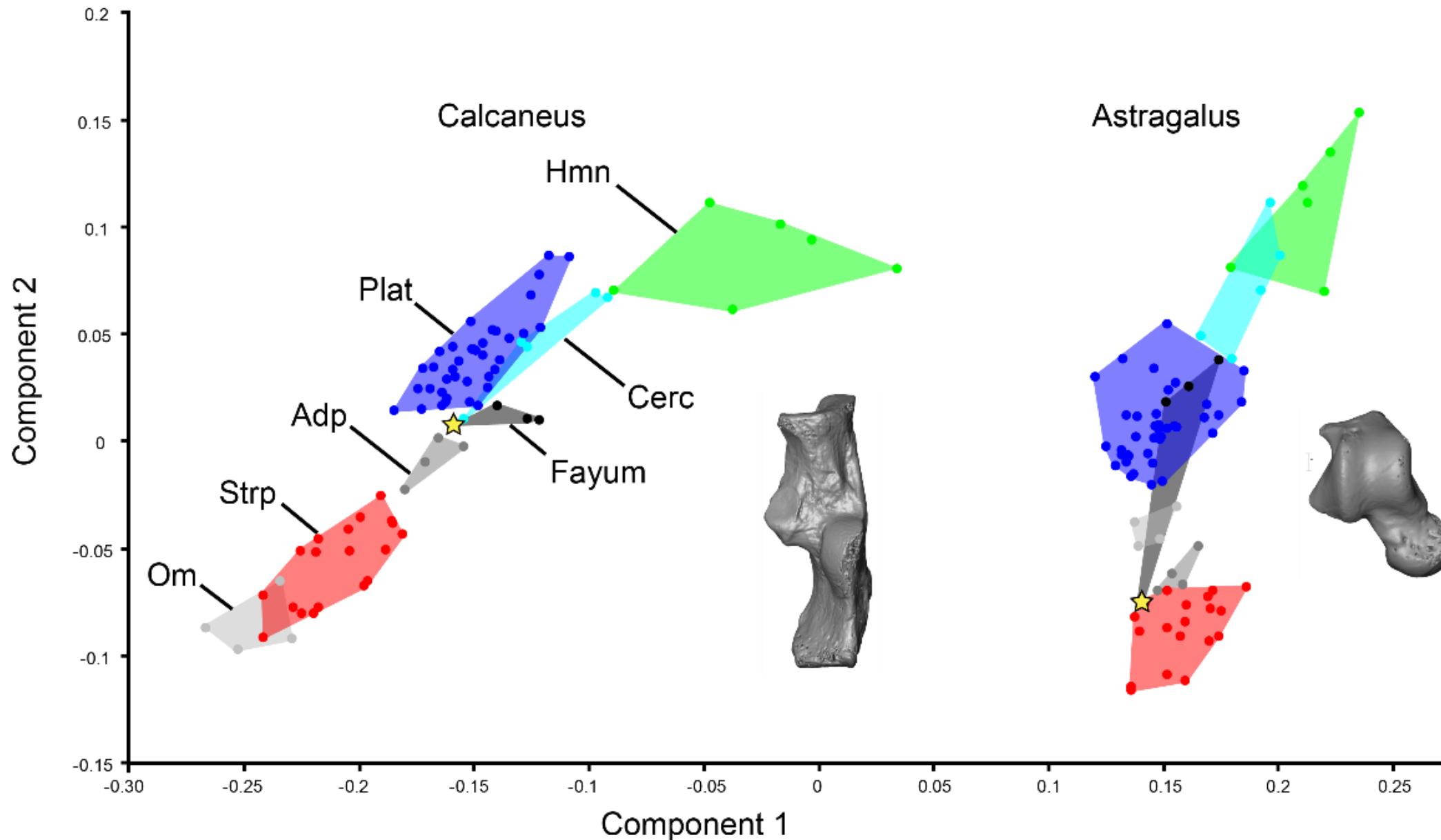
- Combined distance matrix
 - Procrustes alignment and PCA can be run on mixed bone sample

Example

- 80 calcanei and 80 astragali
 - Taxon matched
 - Stats
 - Compare morphospace area
 - Proxy for disparity
 - Compare phylogenetic signal
 - Tree from 10k trees website
 - Check for correlations in PCA

PCD matrix

Results



Results

Stats

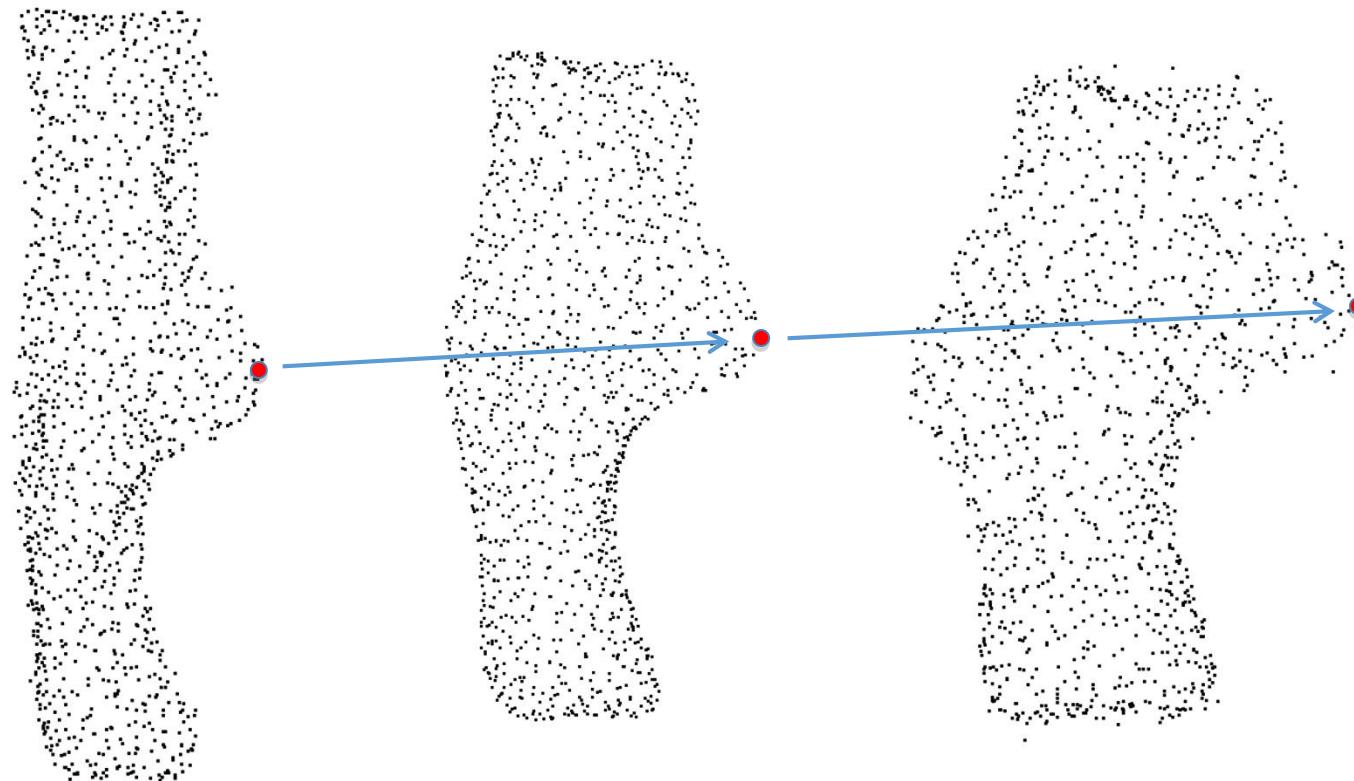
- PC1-2 plot area
 - Calcaneal data occupy 30% more area
- Variance
 - Equal magnitude in calcaneal and astragalar samples
 - Higher magnitude in combined samples
- Phylogenetic signal (Pagel's λ)
 - Higher in calcaneal data than astragalar
 - Higher magnitude in combined samples
- Correlations
 - For a taxon, PC1 score of calcaneus highly correlated with PC1 score of astragalus

Other stuff...

Some other properties/limitations

- Only small deformations allowed (some definitions of homology/correspondences violated)

What we want (?)

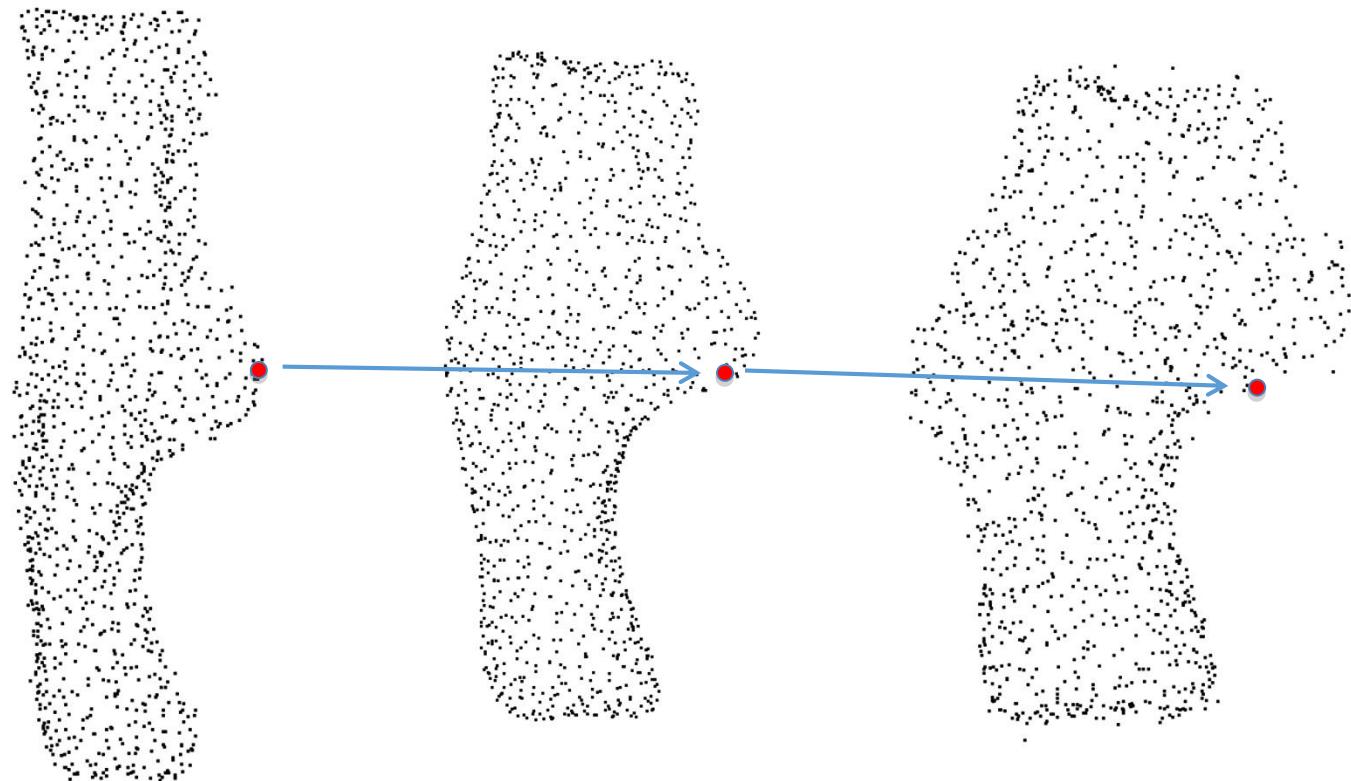


Other stuff...

Some other properties/limitations

- Only small deformations allowed (some definitions of homology/correspondences violated)

What we get (with auto3dgm)



Homology and correspondence

Are they the same thing?

“The same organ in different animals under any variety of form and function” (Owen, 1843)

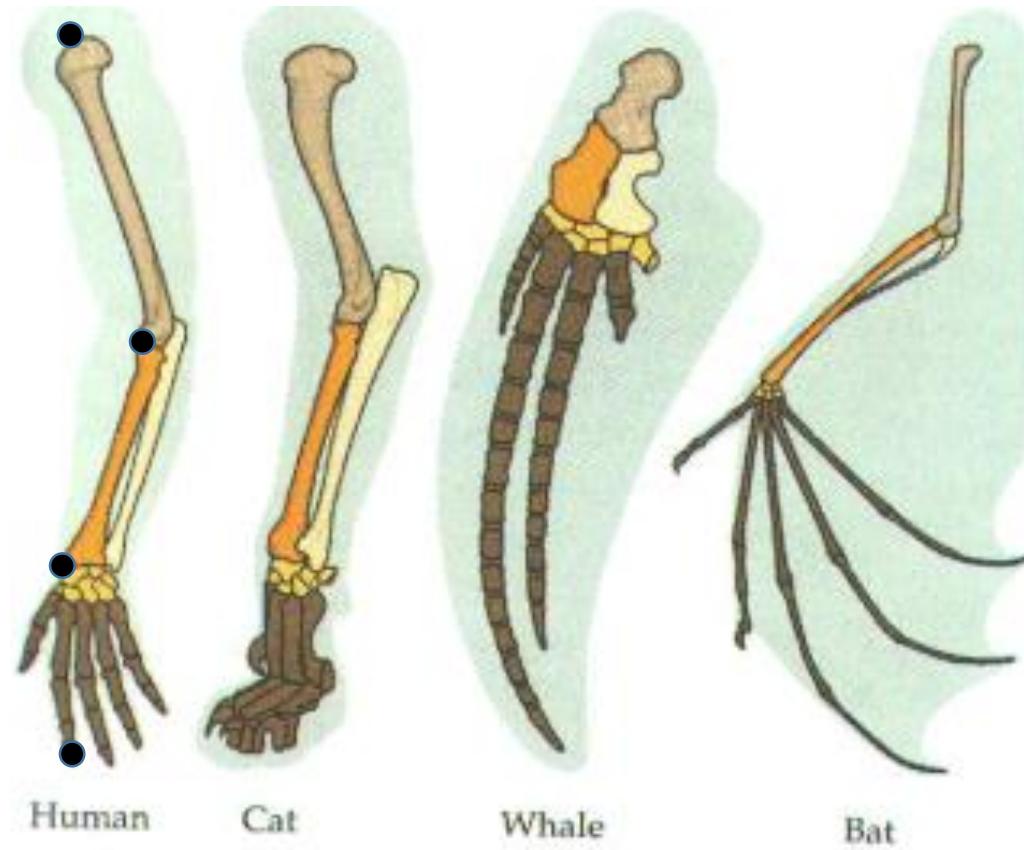
“biological homology refers to unitary structures; not to the infinitesimal coordinate locations on structures that can be defined under the concept of geometric homology” (MacLeod, 2001)

Homology

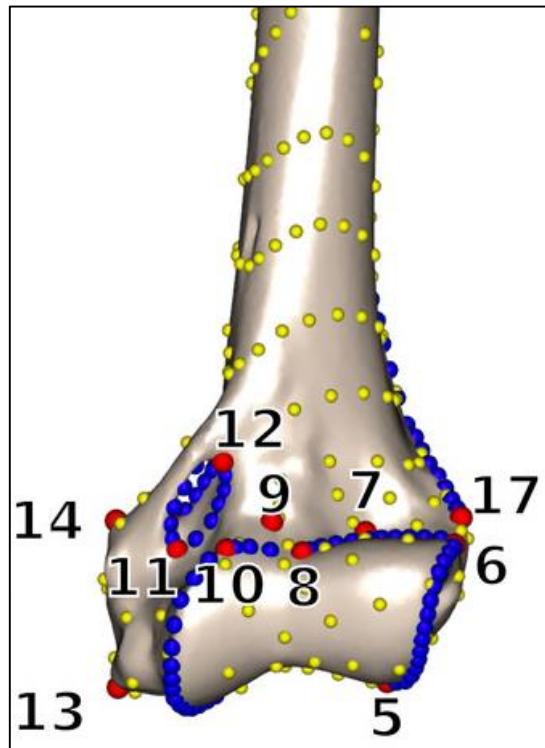
- Kinds of Homology
 - Transformational (aka ‘genealogical’ or ‘Darwinian’)
 - Serial (homologous by developmental duplication)
 - Operational (hypothesis for the purpose of communication or measurement)
 - Taxic (variation in transformational homologous features)

Homology

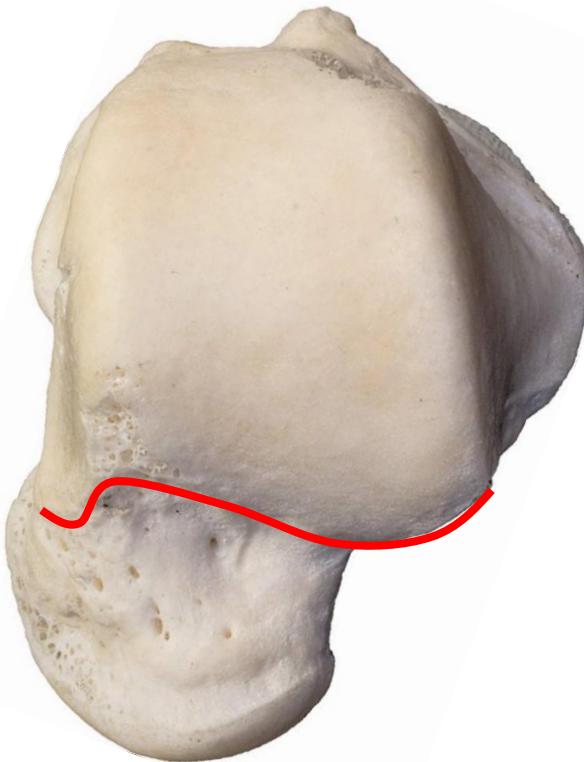
Biological homology & geometric homology converge nicely in a skull



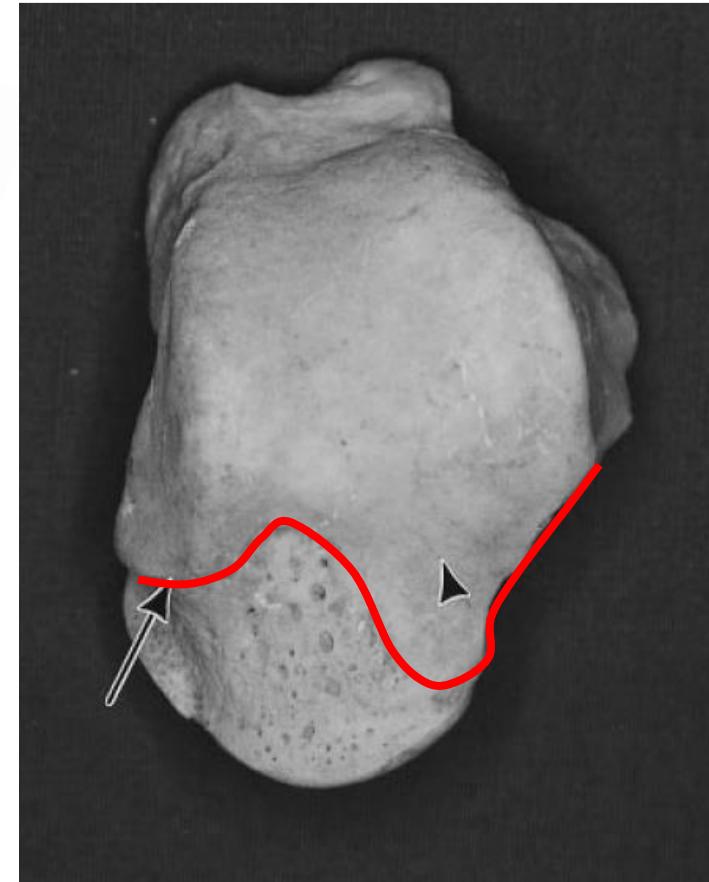
Homology of facet boundaries as ‘type 1’



Left humerus, distal end,
anterior view
Bonn-Divett et al. (2019)

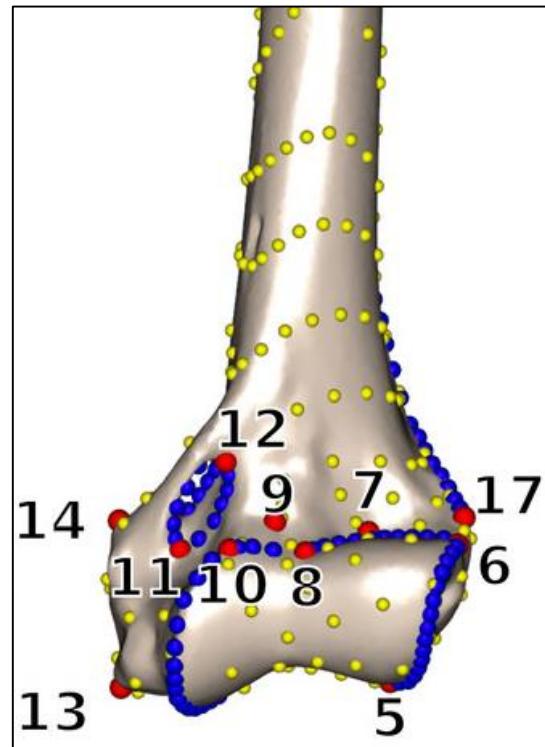


Left talus, dorsal view

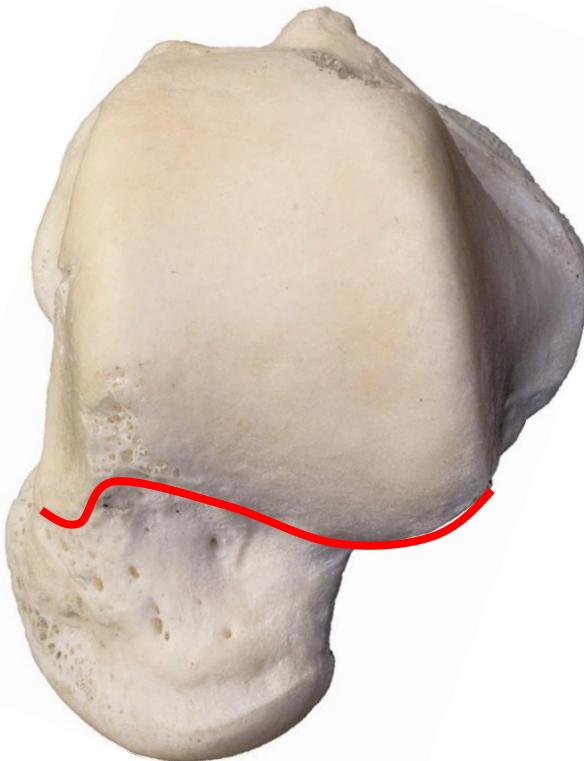


Barnet (1954)

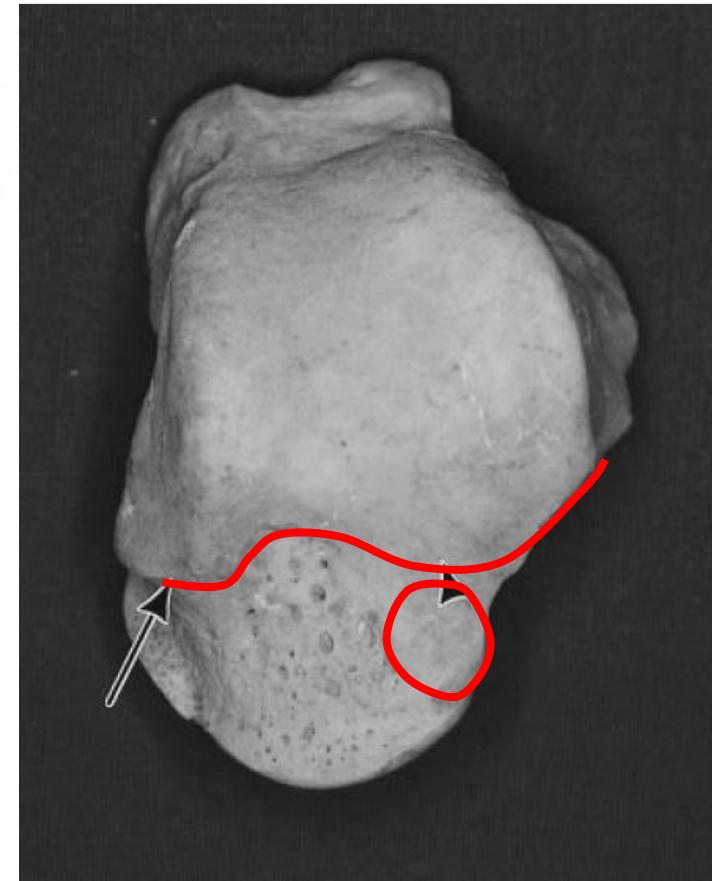
Homology of facet boundaries as ‘Type 1’



Left humerus, distal end,
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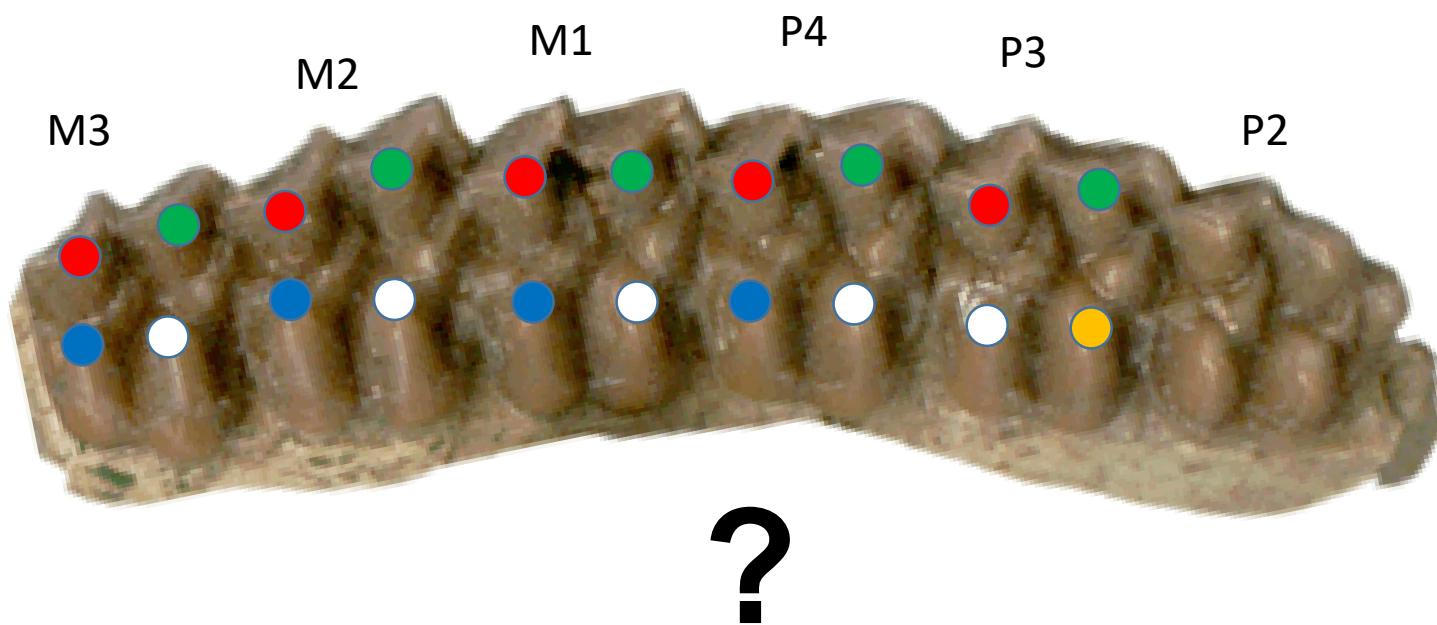
Left talus, dorsal view



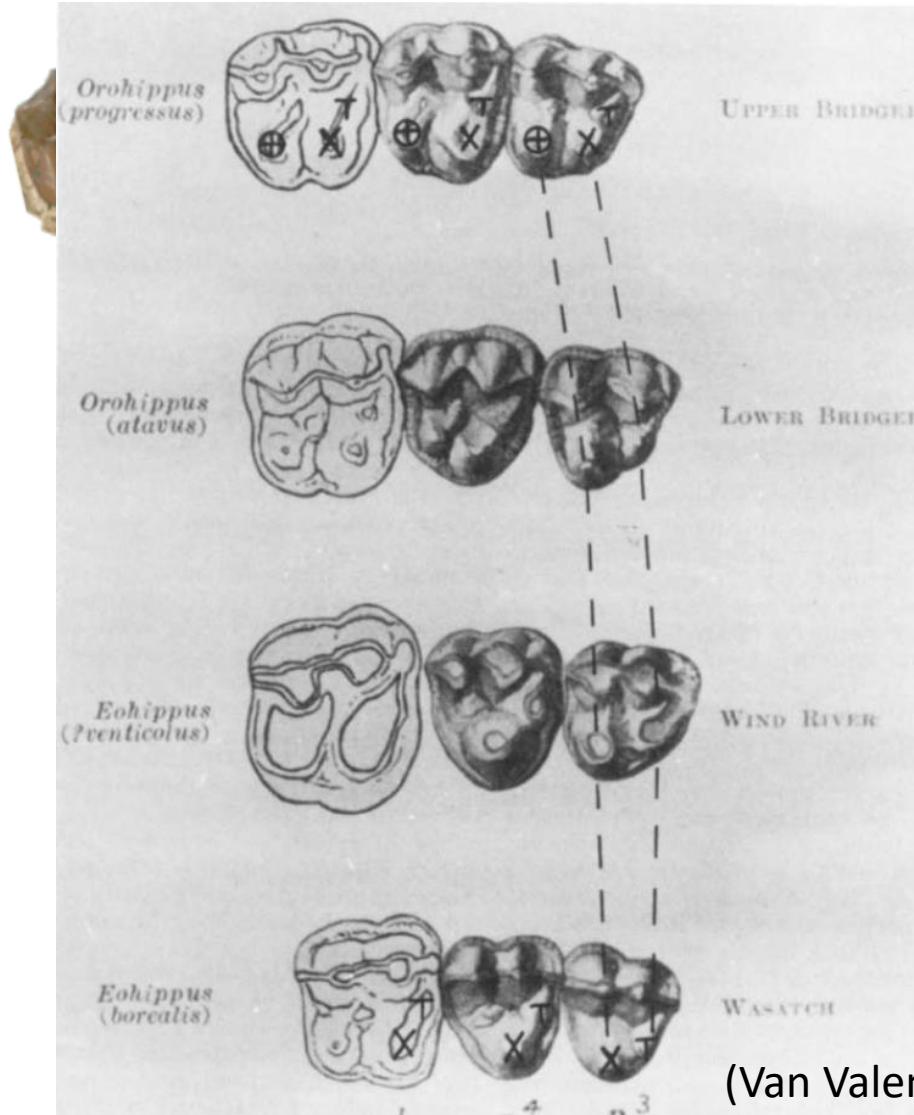
Barnet (1954)

?

Homology of tooth cusps



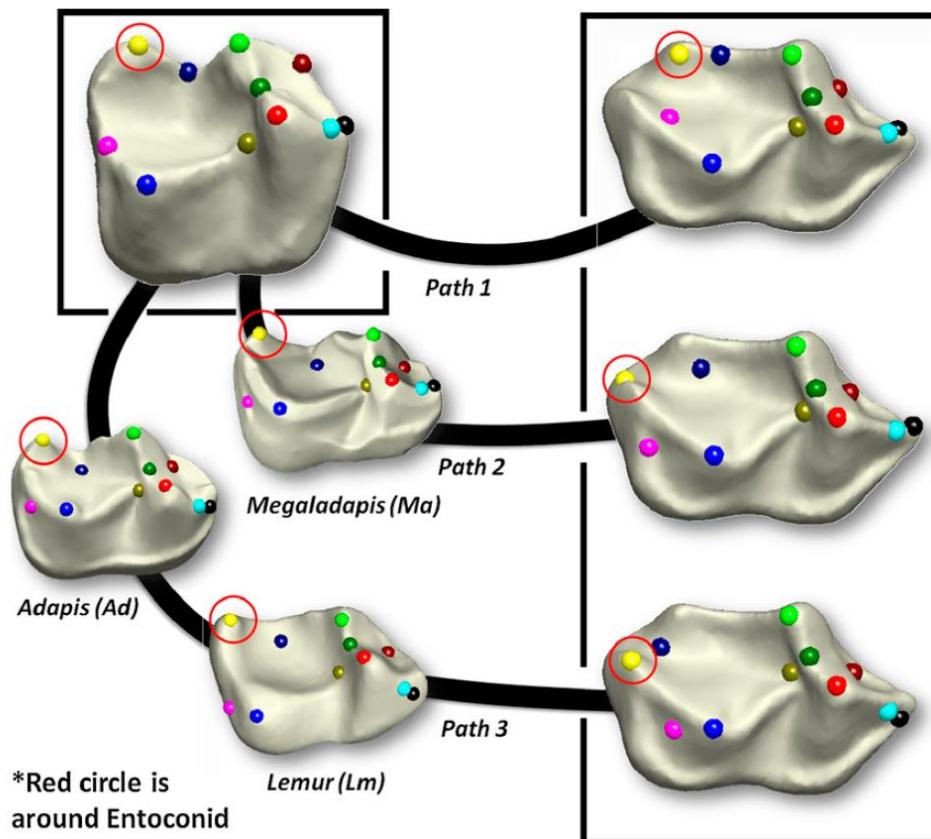
Homology of tooth cusps



- Homology & correspondence interpretations are influenced by sample & the inferred relationships of species in it.
- Therefore, correspondence hypotheses should emerge from analyses, not be predetermined.

On the horizon

- Feature-aware mappings that are transitive

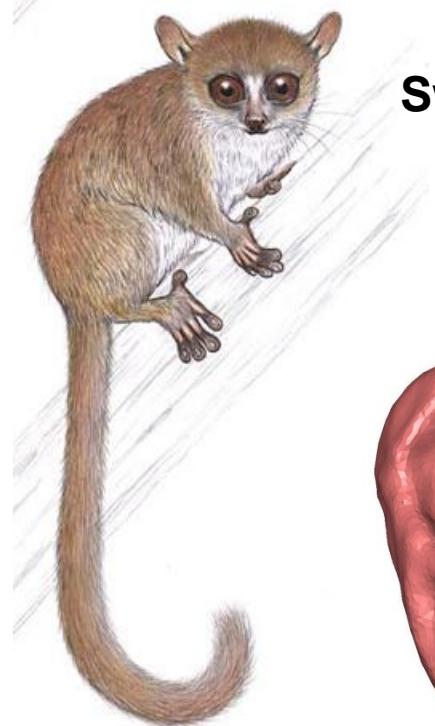


*Red circle is
around Entoconid

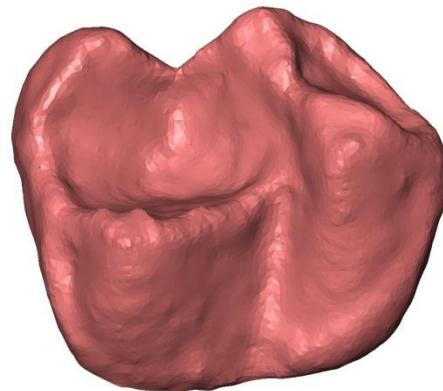
On the horizon

- Feature-aware mappings that are transitive
- Probabilistic correspondence
 - Identify and compare ‘corresponding regions’ rather than points
 - Entertain mappings where ‘regions’ are lost or gained (i.e., not all regions need to be present in every object).
 - Could resolve issues identified for using GM in phylogenetic analysis (e.g, MacLoed, 2001)

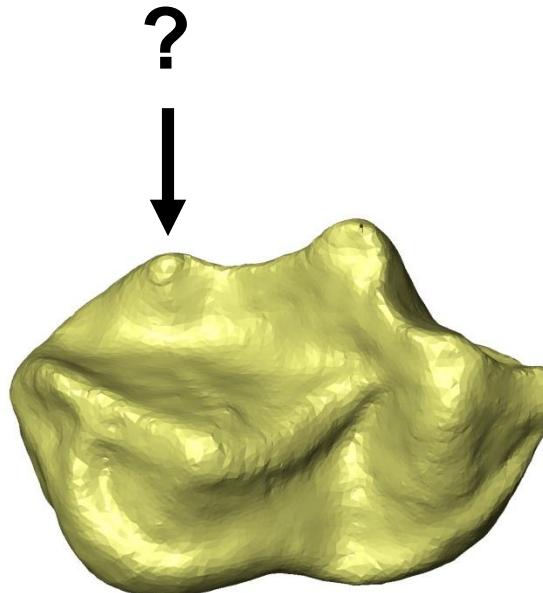
Disputed homologies in *Lepilemur*



Swindler 2004



Microcebus



Lepilemur

?

↓

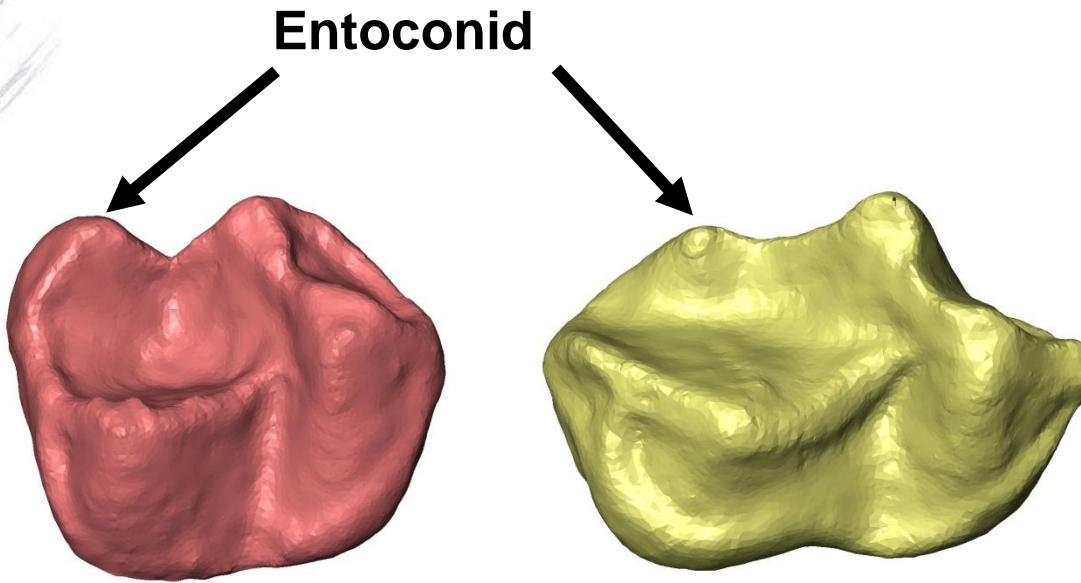


Boyer et al. 2011 (PNAS)

Disputed homologies in *Lepilemur*



Swindler 2004



Microcebus

Lepilemur

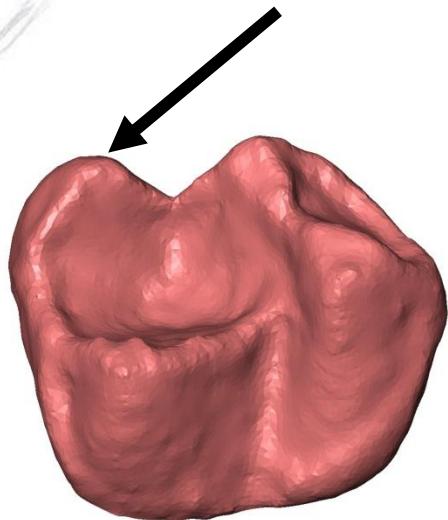


Disputed homologies in *Lepilemur*



Swindler 2004

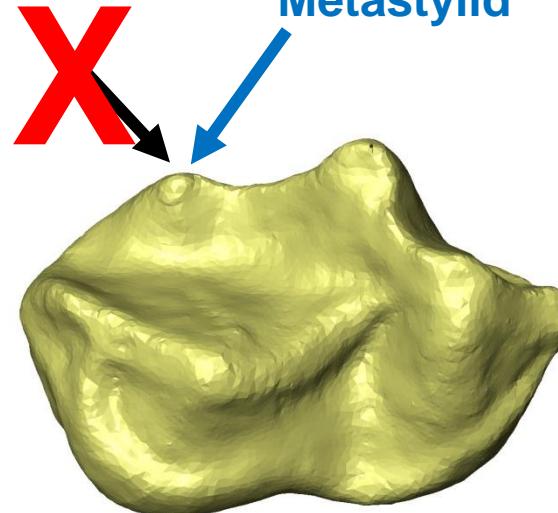
Entoconid



Microcebus

Schwartz & Tattersall 1985

Metastylid



Lepilemur

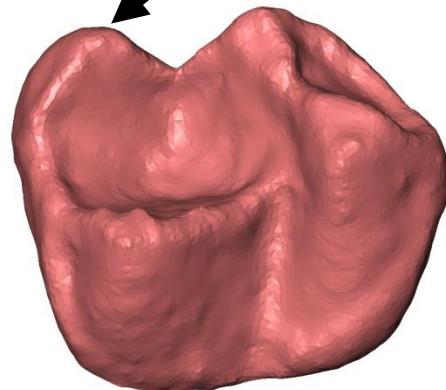


Why the difference?



Swindler 2004

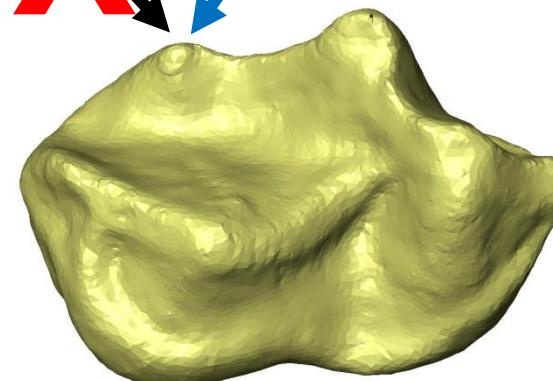
Entoconid



Microcebus

Schwartz & Tattersall 1985

Metastylid



Lepilemur

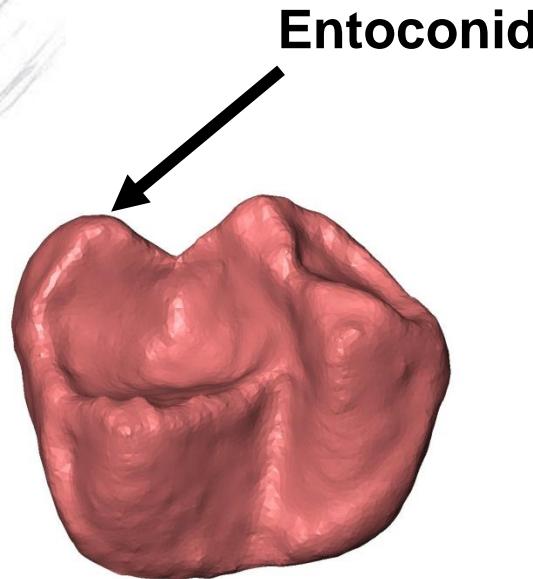


Comparisons to a different taxon

Megaladapis

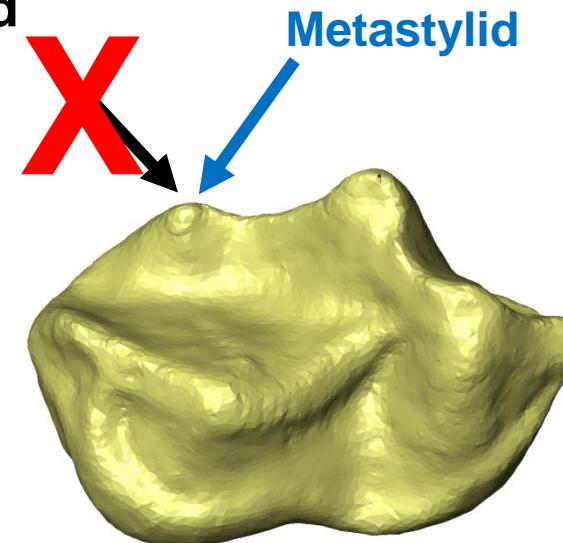


Swindler 2004



Microcebus

Schwartz & Tattersall 1985

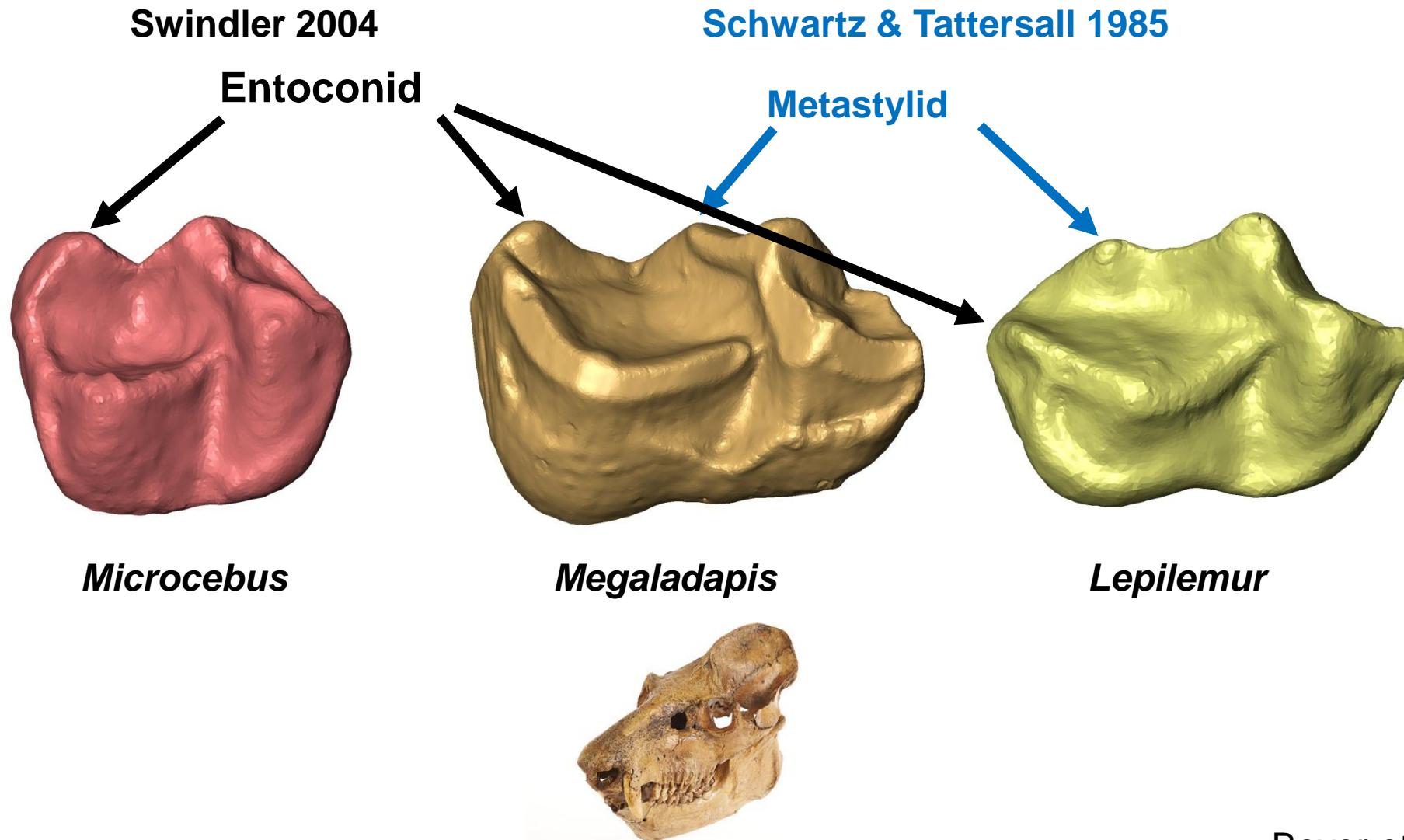


Lepilemur

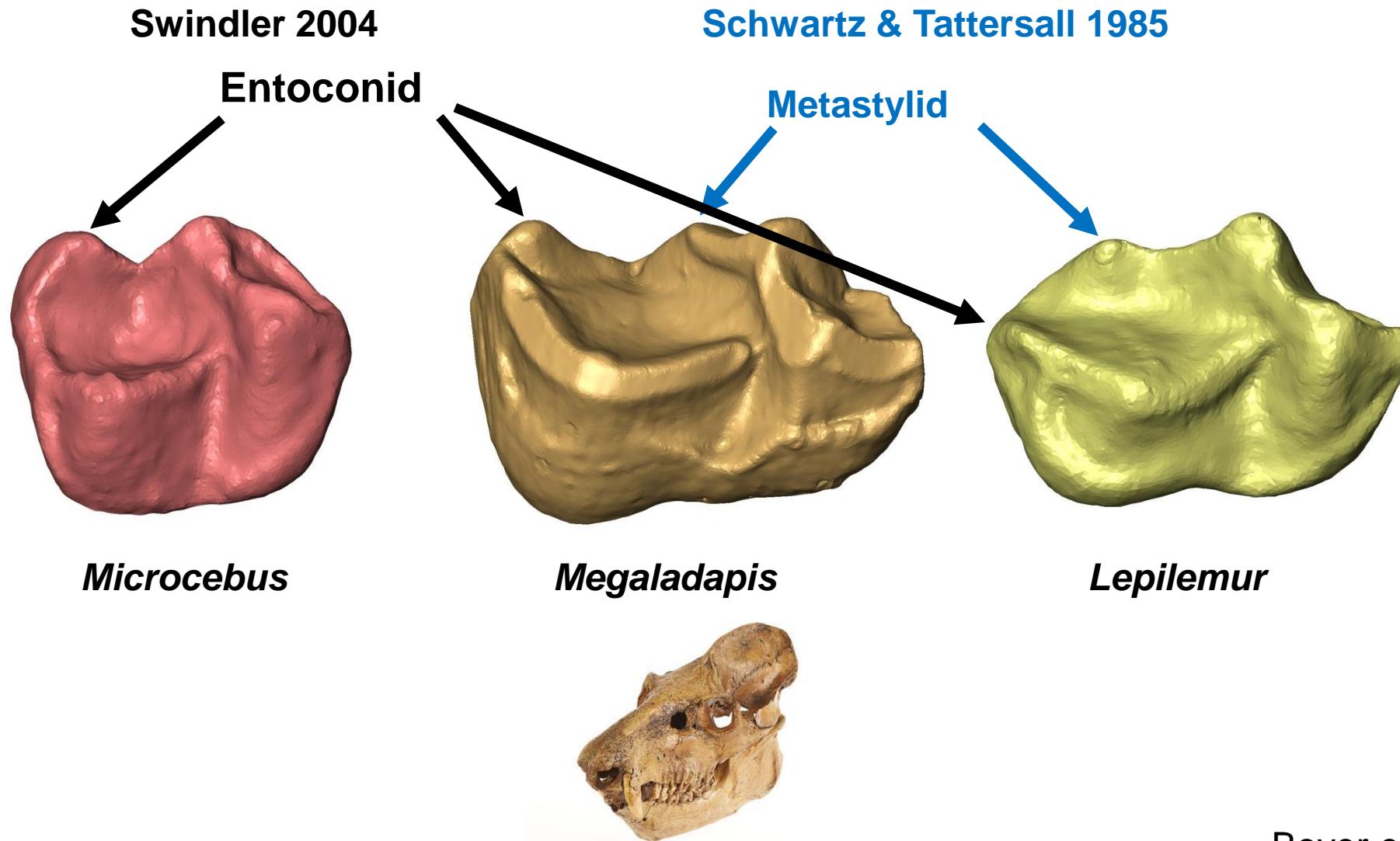


Comparisons to a different taxon

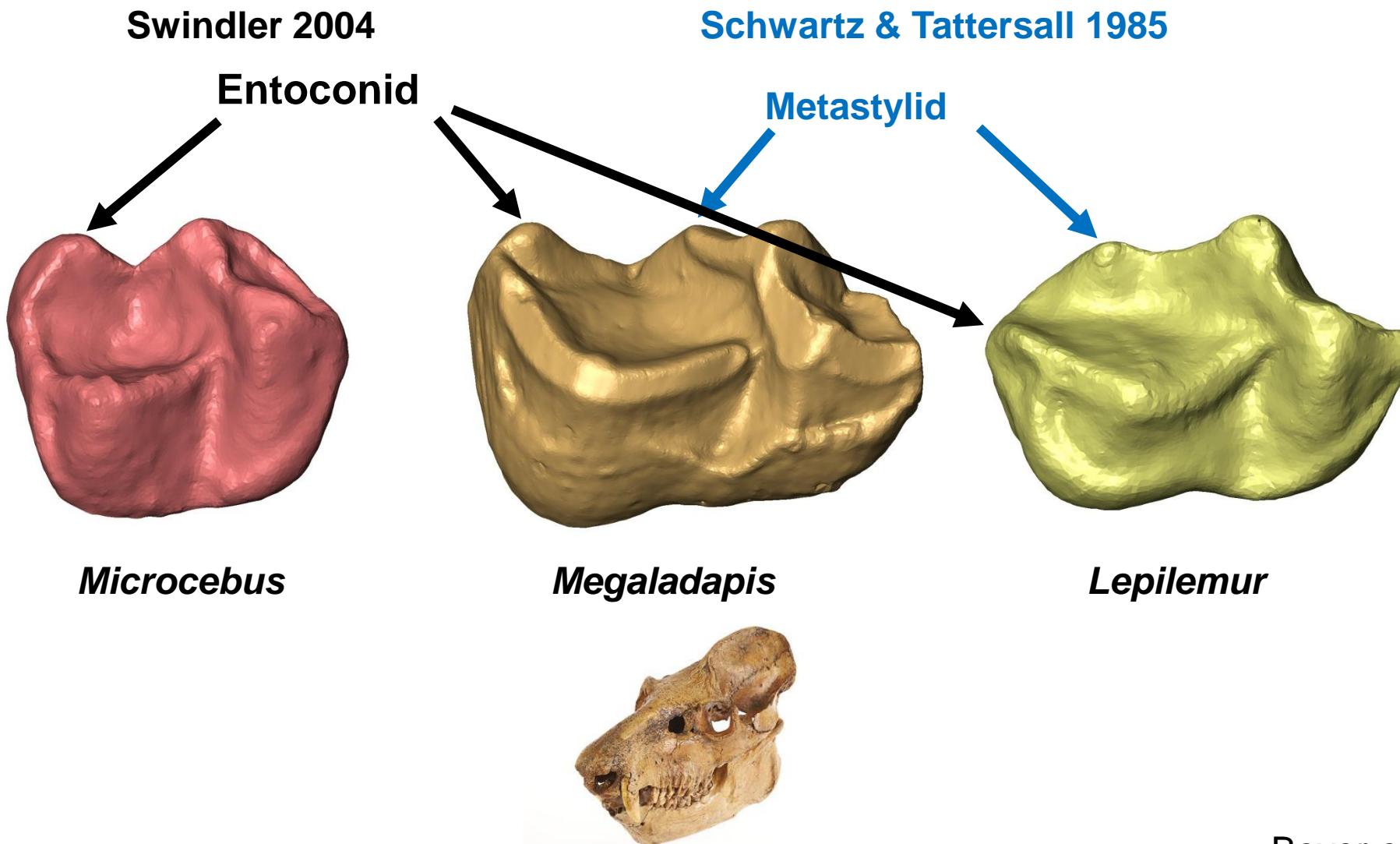
Megaladapis



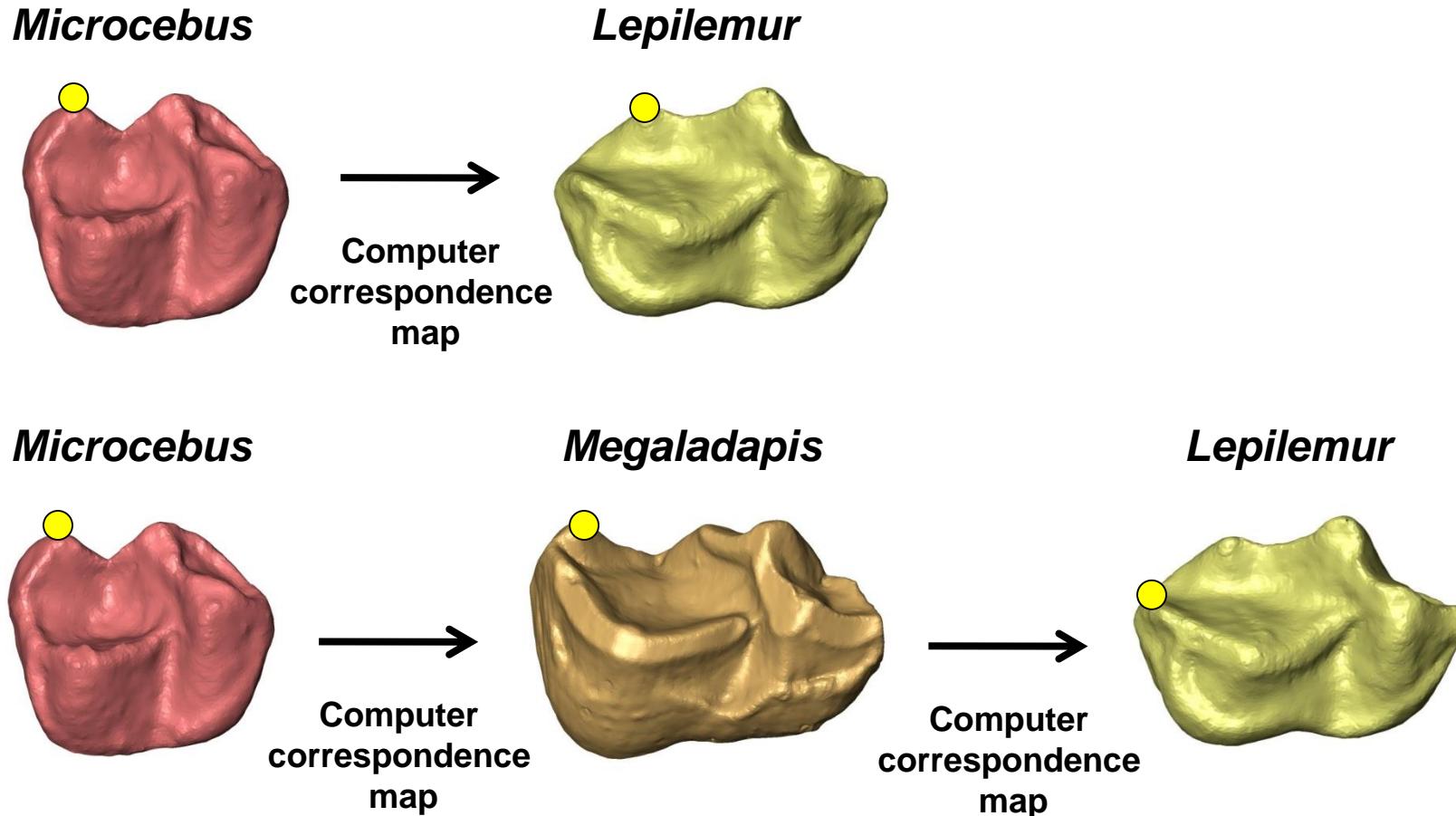
Correspondence id's must not be static



Does comparative sample affect algorithm's homology identification?



Does comparative sample affect algorithm's homology identification?



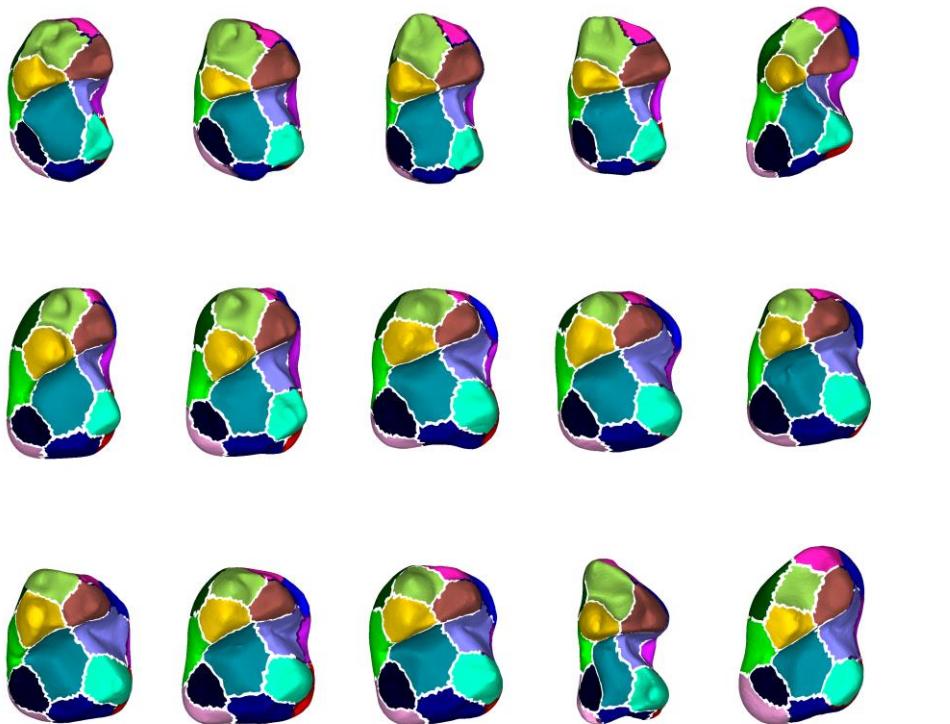
Significance?

- Automated correspondence allows tests of homology hypotheses that are influenced by hypothesized transformational series or phylogenies.
- Propagating correspondence according to such a series may give more meaningful sense of shape variation in post hoc ordinations of correspondence data.

Probabilistic correspondence

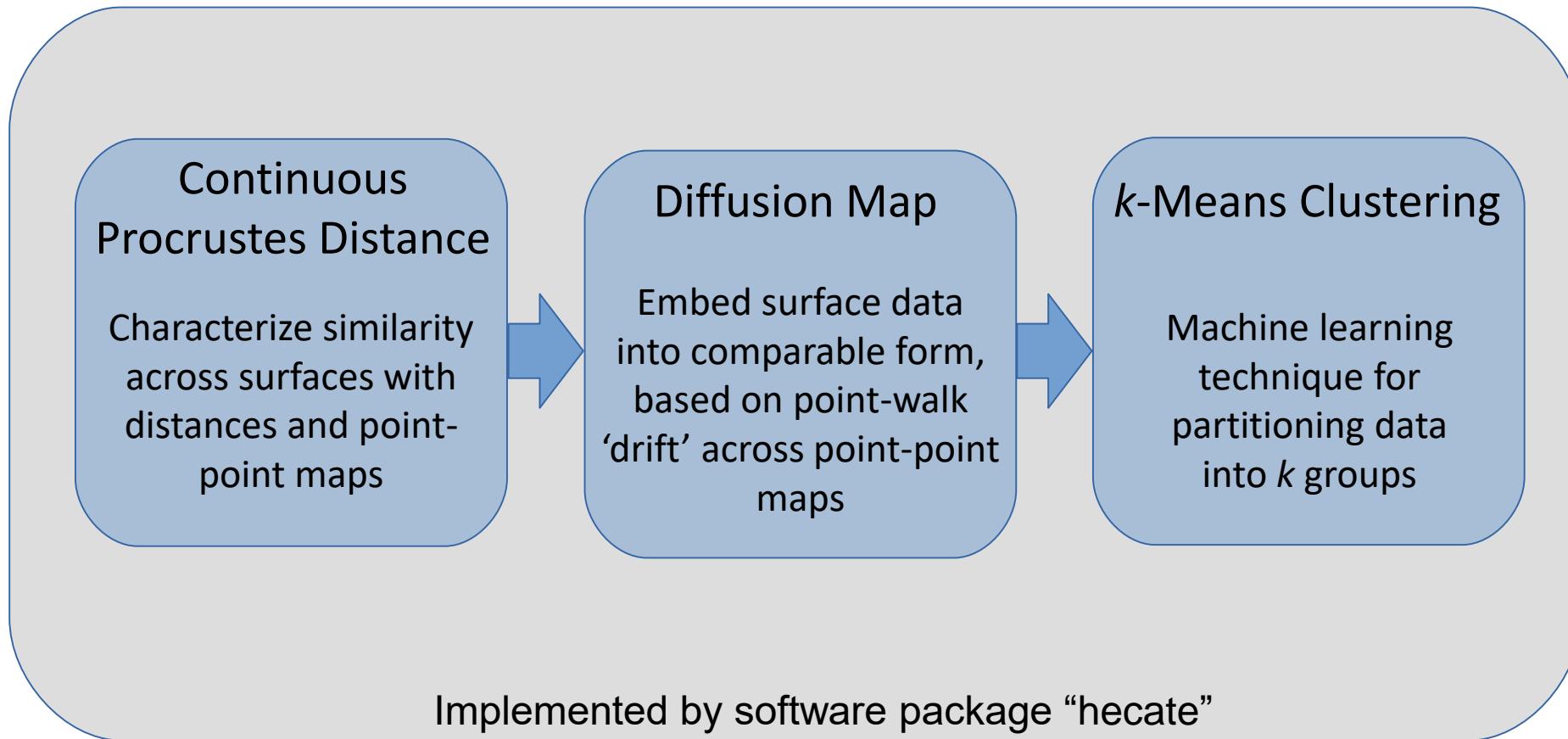
“As biologists, our objective in choosing landmarks is to permit making inferences about the regions between them—we are not interested in the landmarks *per se*, but in the shapes of the morphological structures on which those landmarks lie.” (Zelditch et al. 1995)

Diffusing surfaces to model evolution of form

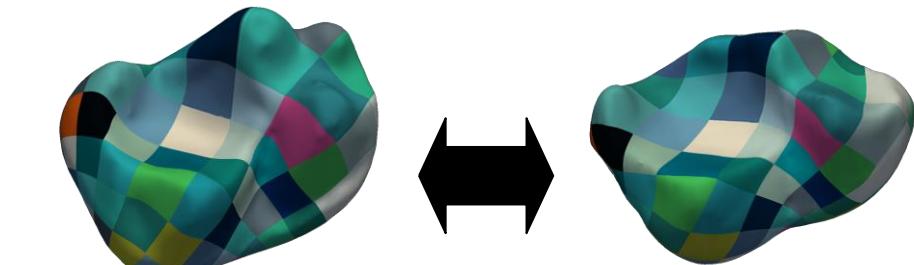


- Attempt to objectively recognize discrete surface region ‘characters’

Segmentation method

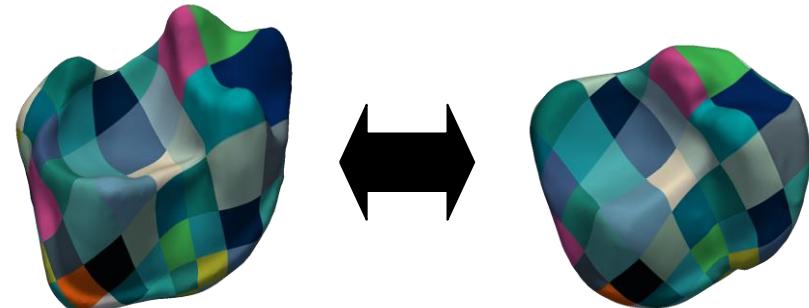


Continuous procrustes distance



Donrusselia gallica

Lemur catta



Tarsius spectrum

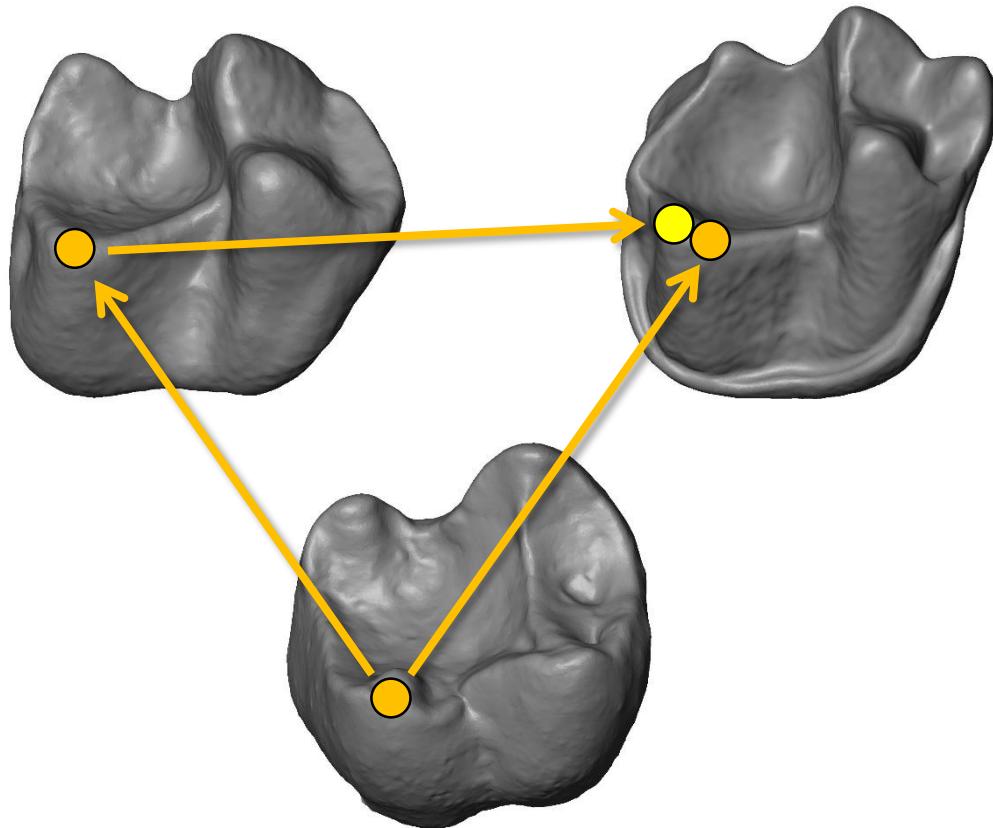
Mirza coquereli

Mesh Continuous
Procrustes
Distances

	A	B	C	D
A		.2	.7	.1
B	.2		.3	.4
C	.7	.3		.5
D	.1	.4	.5	

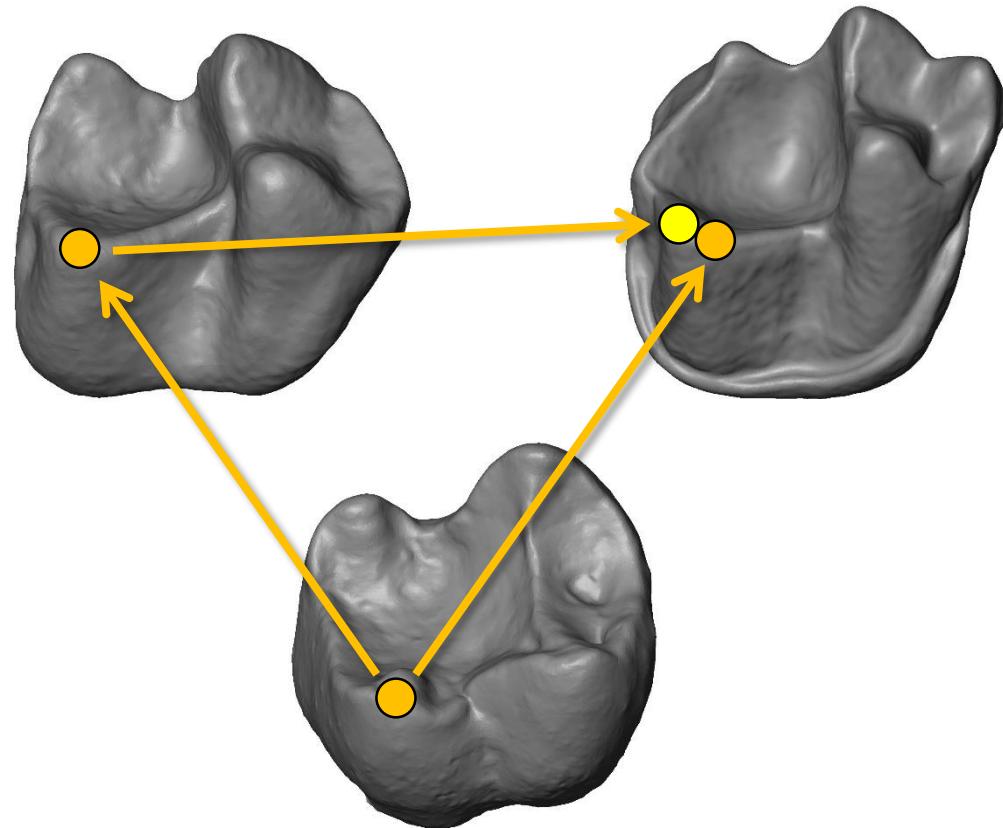
- Produces surface point-to-point correspondence maps and mesh-to-mesh distances

Continuous Procrustes distance



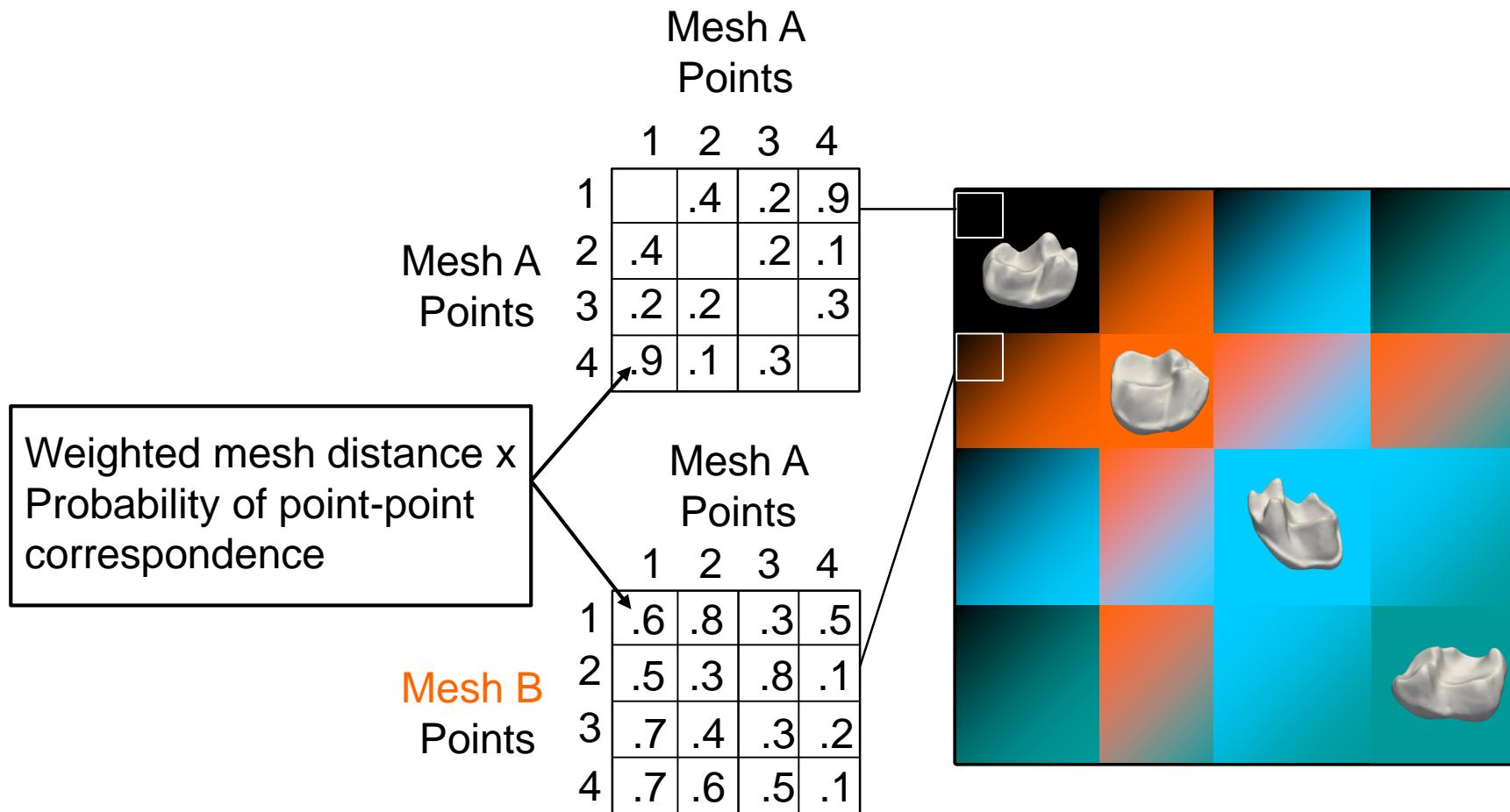
- Possible concern: ‘walking’ point drifts across combinations of surface maps

Continuous procrustes distance



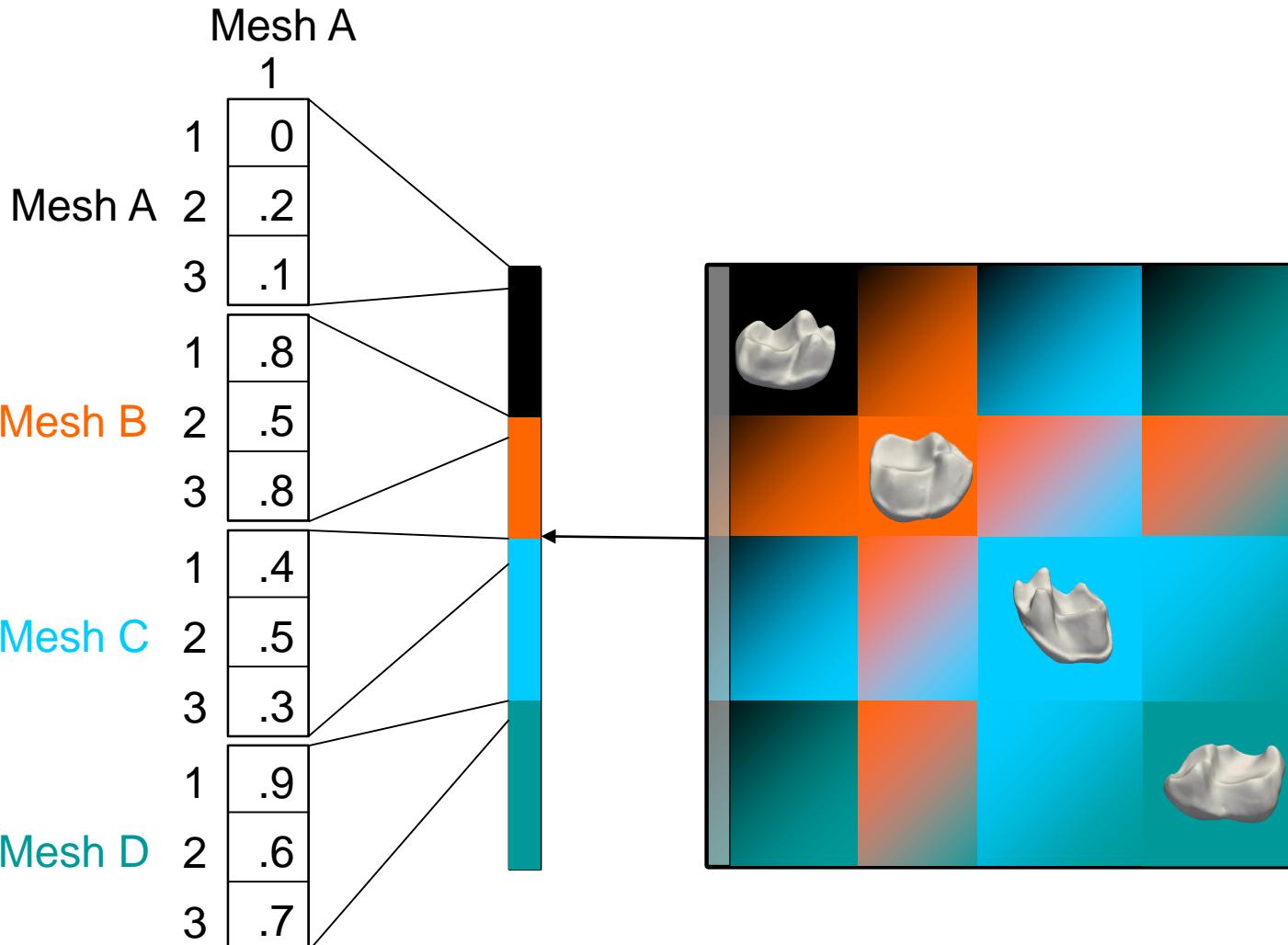
- Positive consequence: In locally similar regions, points likely walk in same ‘neighborhood’

Diffusion operator



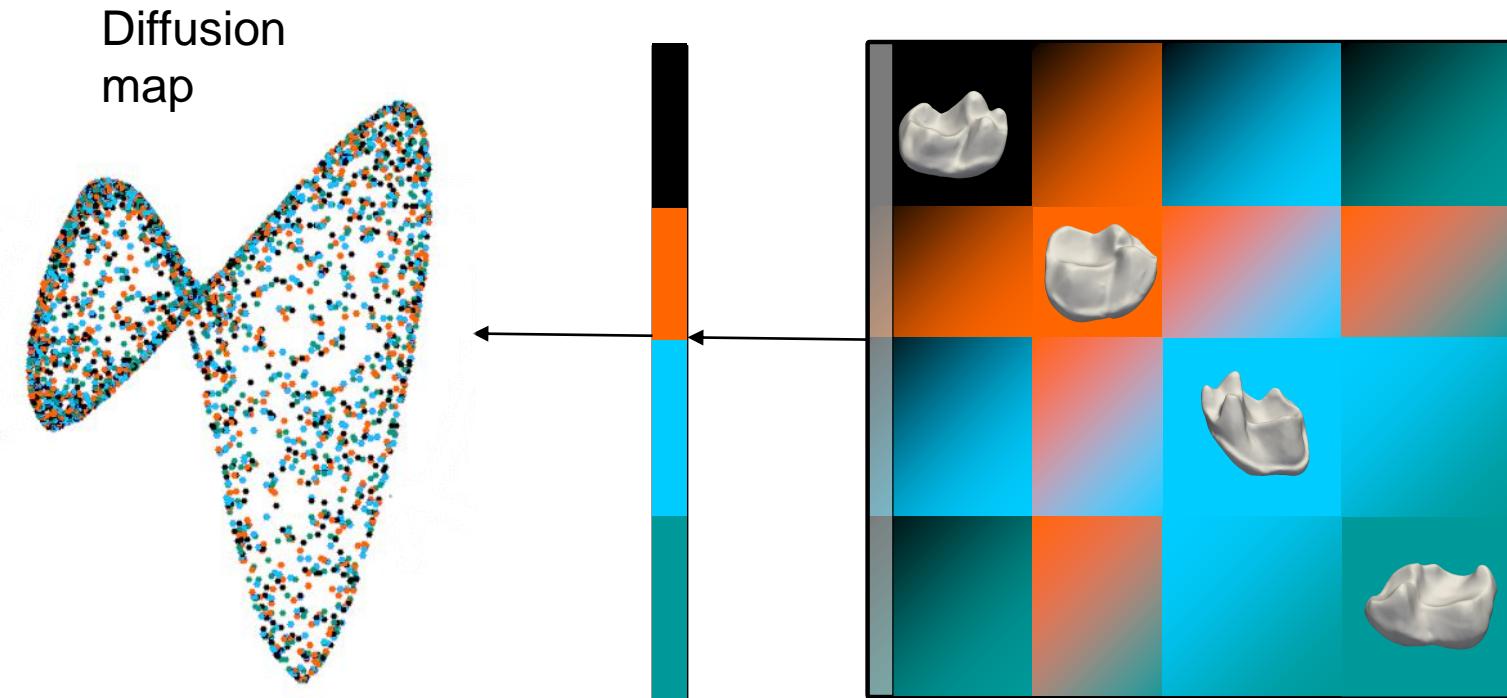
- Matrix comparing **all** points of **all** meshes in sample

Diffusion operator



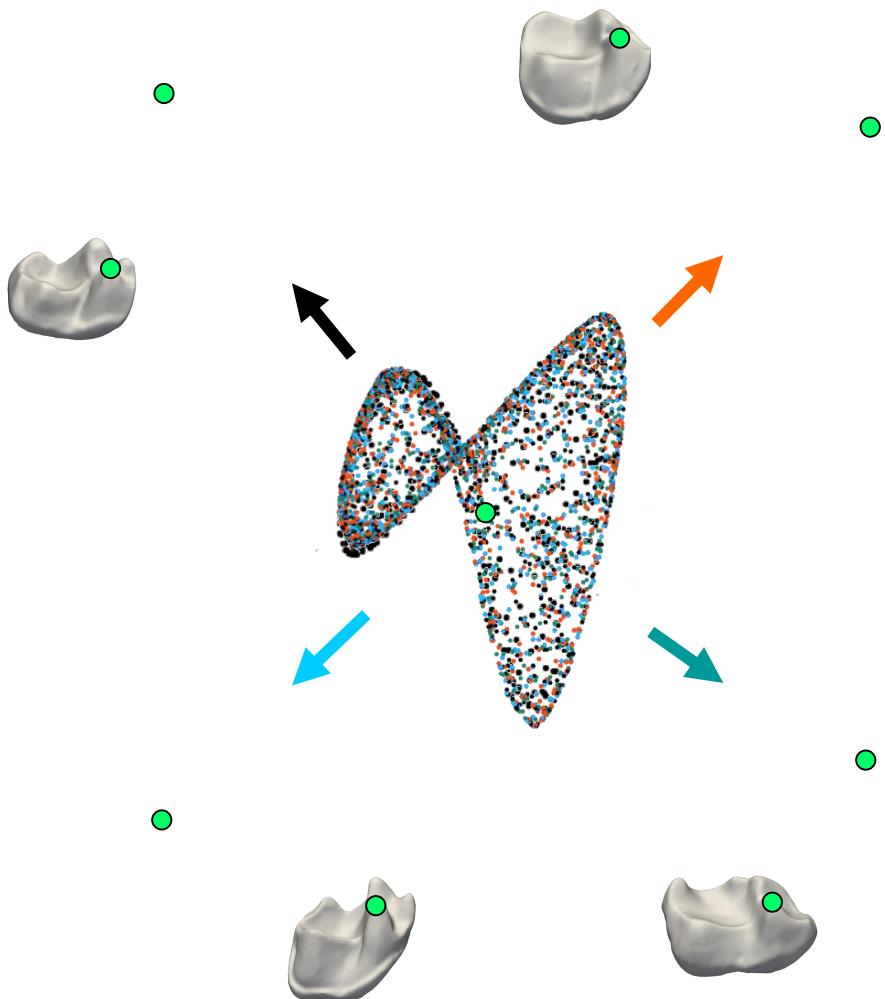
- Matrix column: Single point compared to **all** other points from **all** meshes (including its own)

Diffusion operator



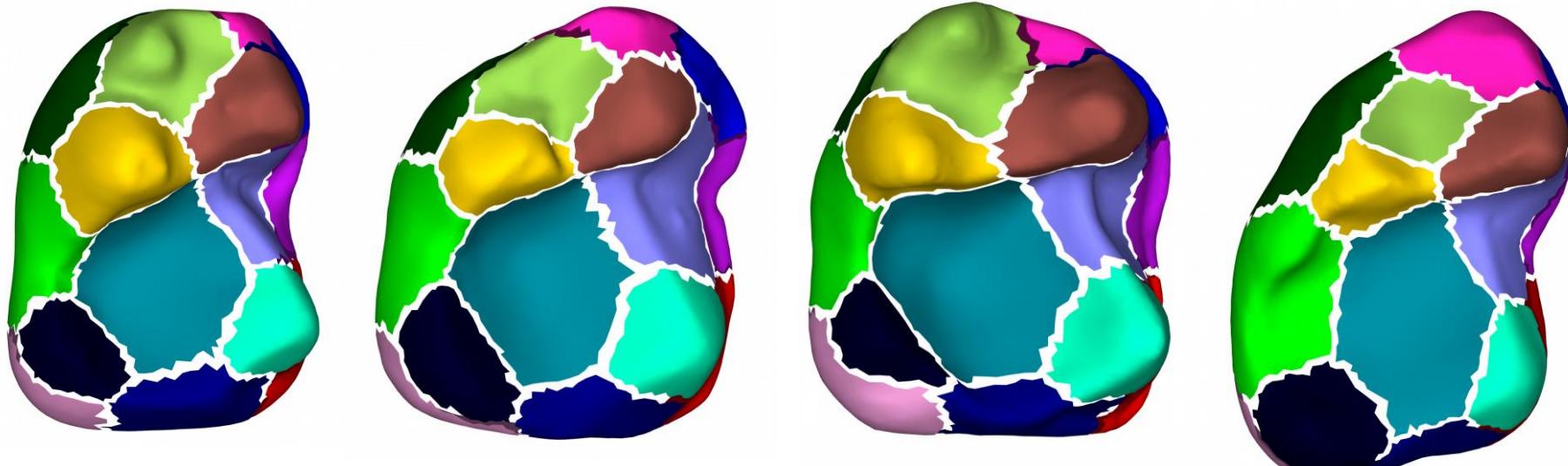
- Matrix column: Single point compared to **all** other points from **all** meshes (including its own)

Diffusion map



- Diffusion map coordinates embed mesh data in new multidimensional space
- Mesh data now similar in form
- Nearness in diffusion map = similarity across original surfaces

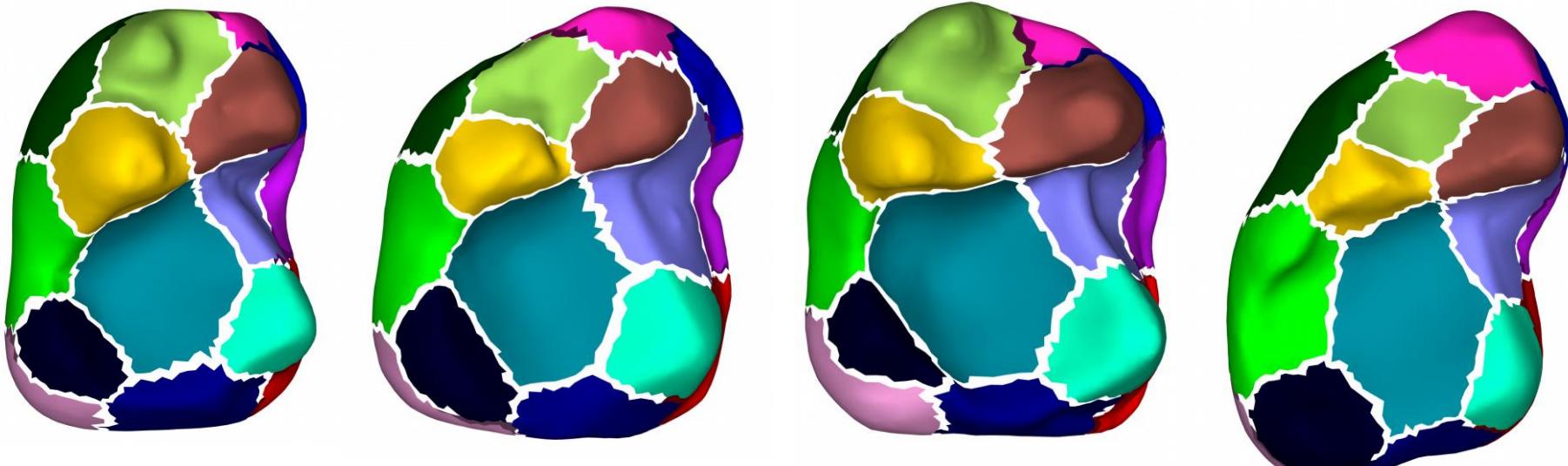
k -Means Clustering



$$k = 15$$

- Partition diffusion map coordinates into k groups, translate to original surface coordinates

k -Means Clustering

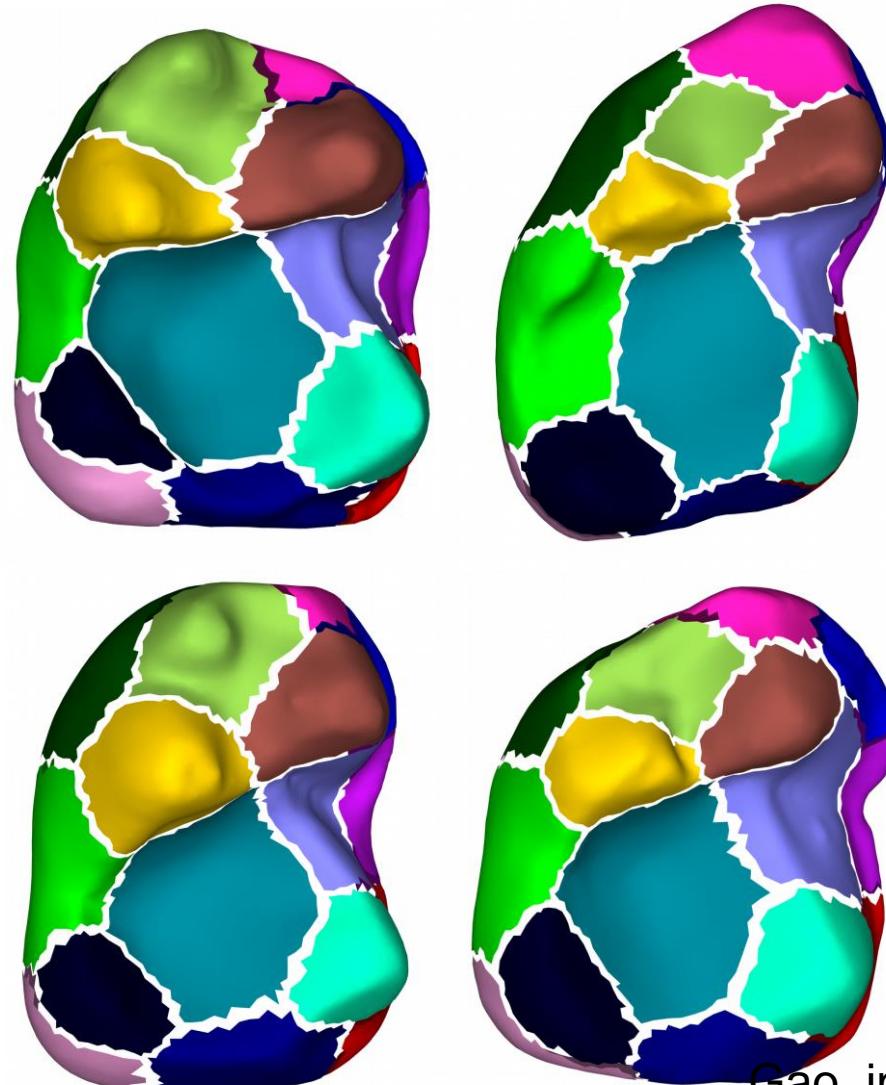


$k = 15$

- Regions reflect local similarity based on probability of walking point ‘drift’ on surface maps

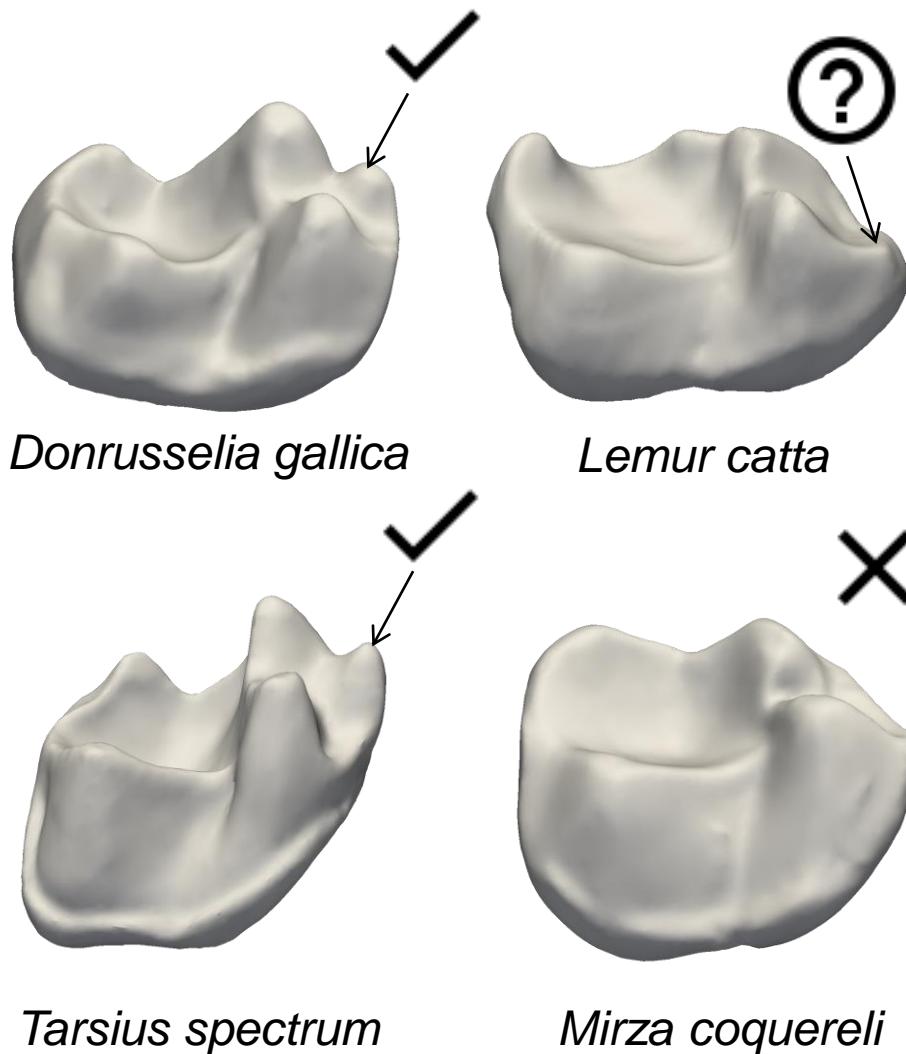
Segmentation results

- Surface regions ($k = 15$) capture major features
 - Cusps
 - Basins
 - Side walls
- Surface feature presence/absence important for questions of taxonomy, phylogeny, function, etc.
- Surface regions may be able to provide an objective quantitative criterion for feature presence



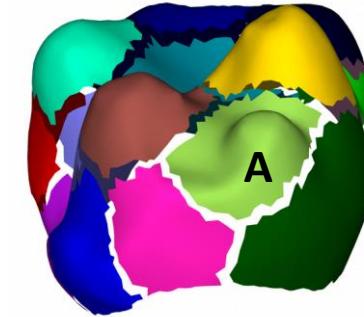
Test: paraconid cusp

- Variable among prosimians
- Qualitative characterizations differ, e.g. *Lemur catta*
 - Ni et al. (2013): weakly present
 - Herrera and Dávalos (2016): absent

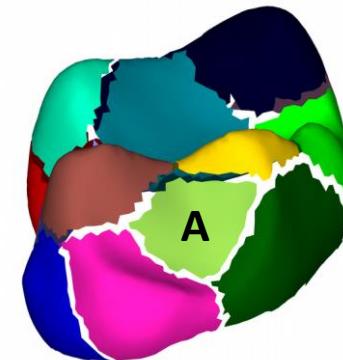


Test: paraconid cusp

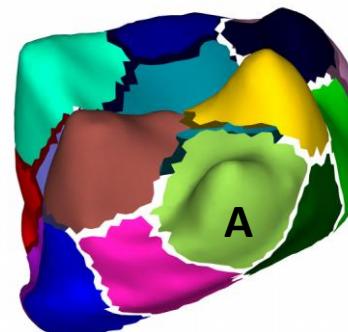
- Sample: 116 prosimian M_2 s, 15 segments
- Species-level paraconid presence/absence
- Quantify surface curvature of segment A
 - Dirichlet normal energy
 - Species means
- Compare groups
 - Welch's T test



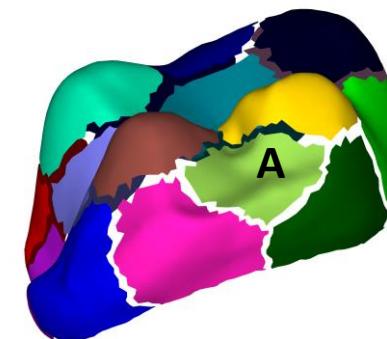
Donrusselia gallica



Lemur catta

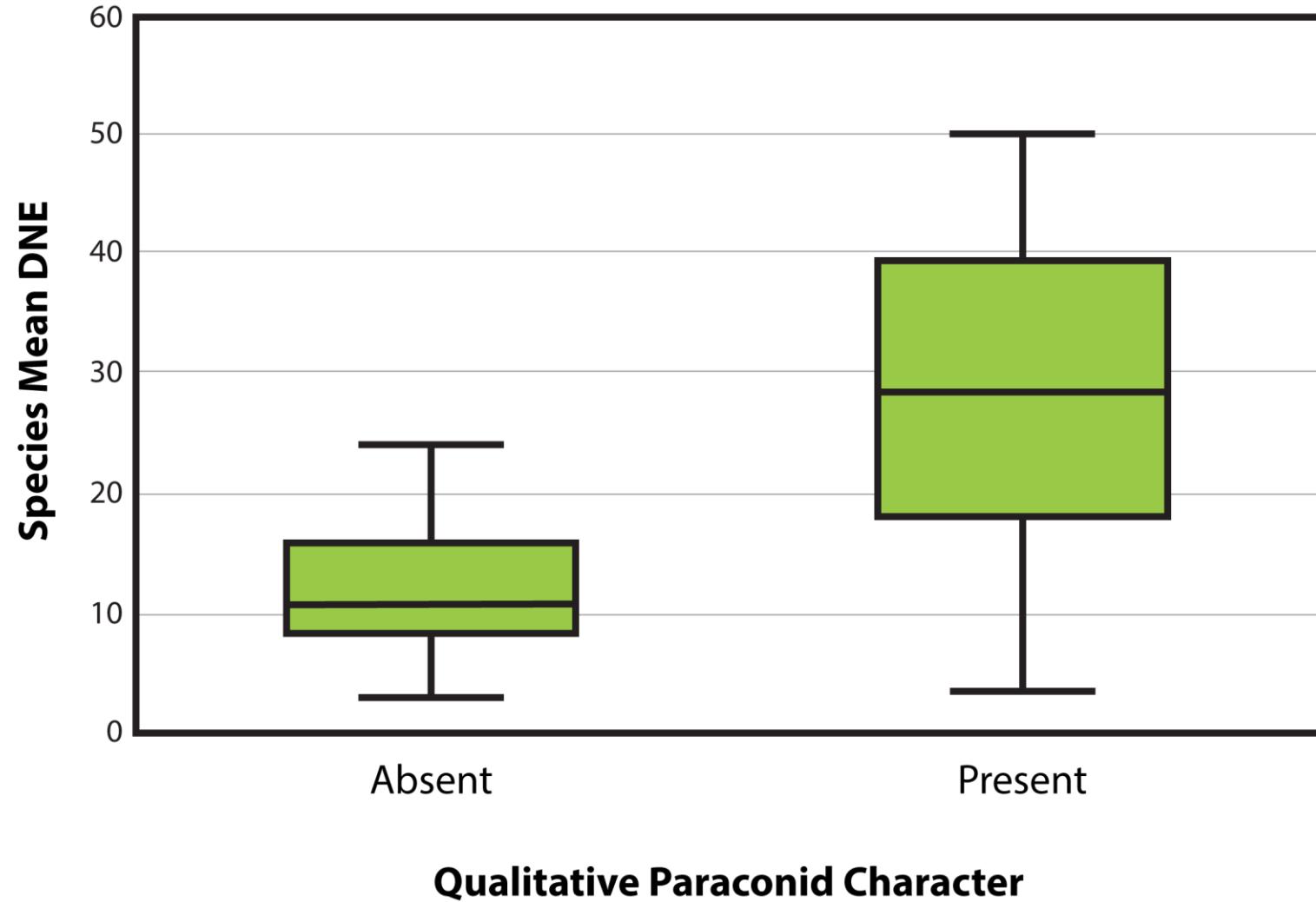


Tarsius spectrum

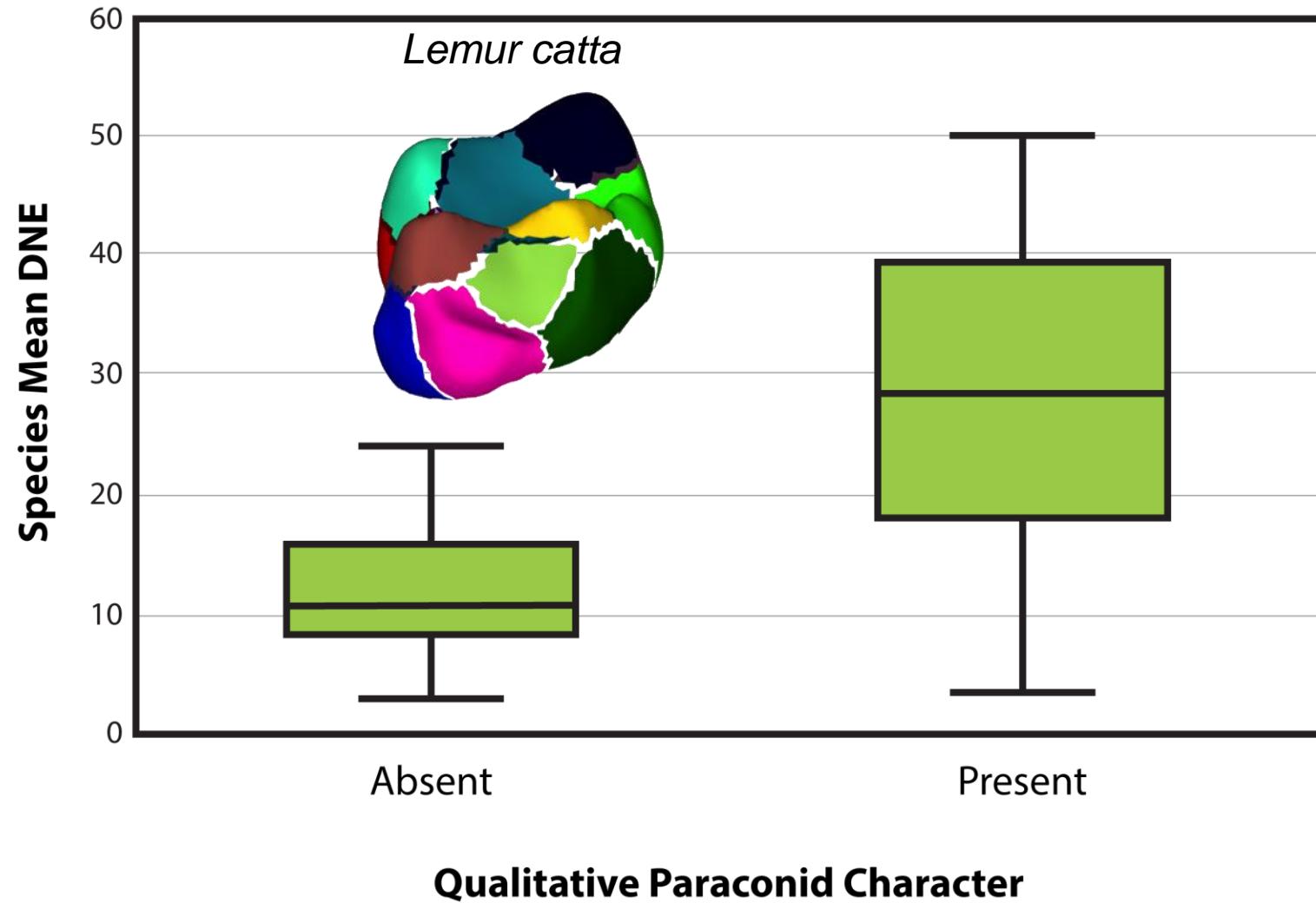


Mirza coquereli

Test: paraconid cusp



Test: paraconid cusp



Test: paraconid cusp

