

Automated Shape Correspondence:

Why and How

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Outline

- Goals & Rationale
- Limitations of traditional landmarks
- Definition of 'automated correspondence' & potential
- *Auto3dgm*: Concepts & Logistics
- Homology and its relationship to correspondence
- Inspiring applications
- Some things to know about Slicer auto3dgm and the demo sample

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.

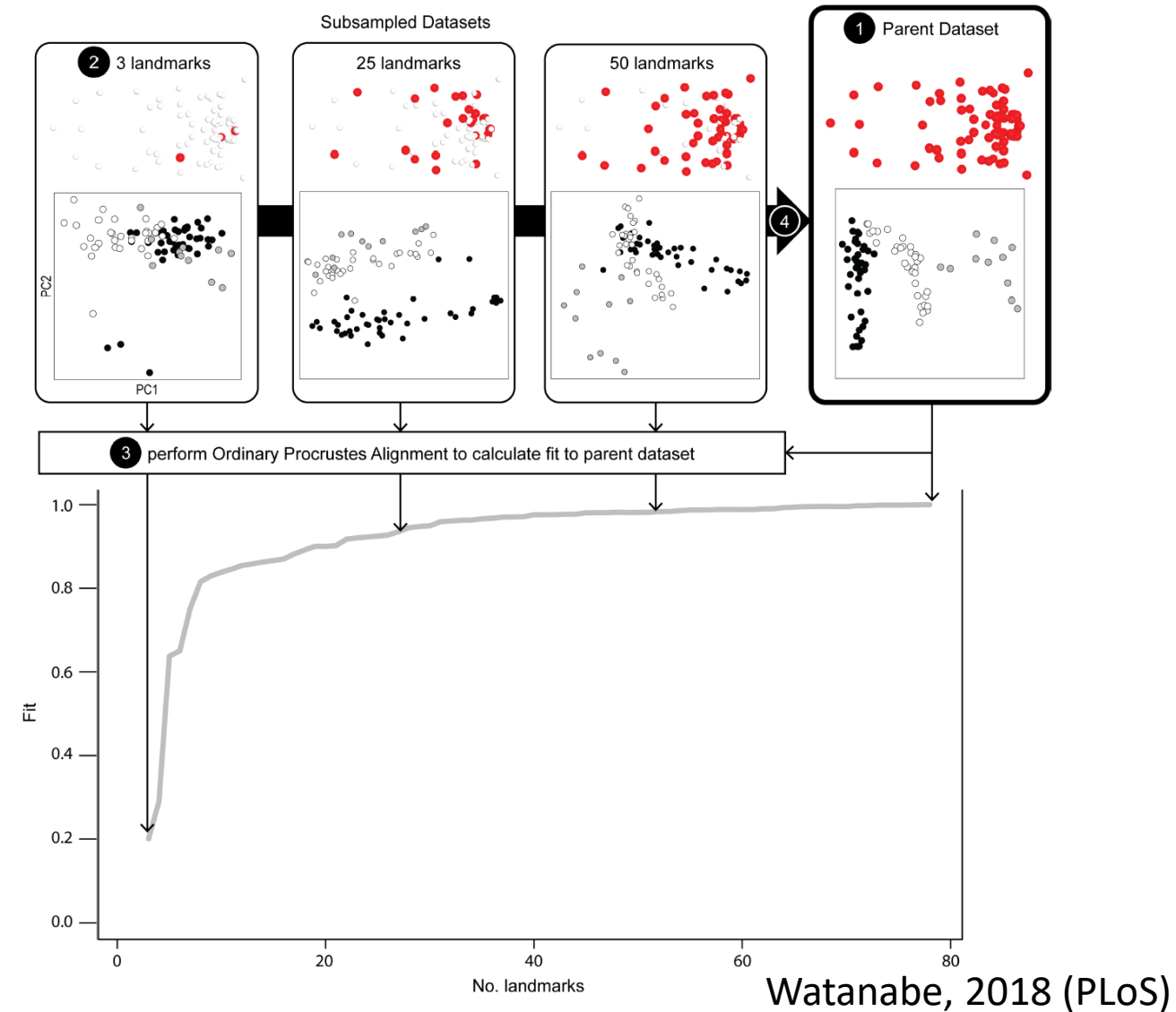
Limitations of traditional landmarks

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



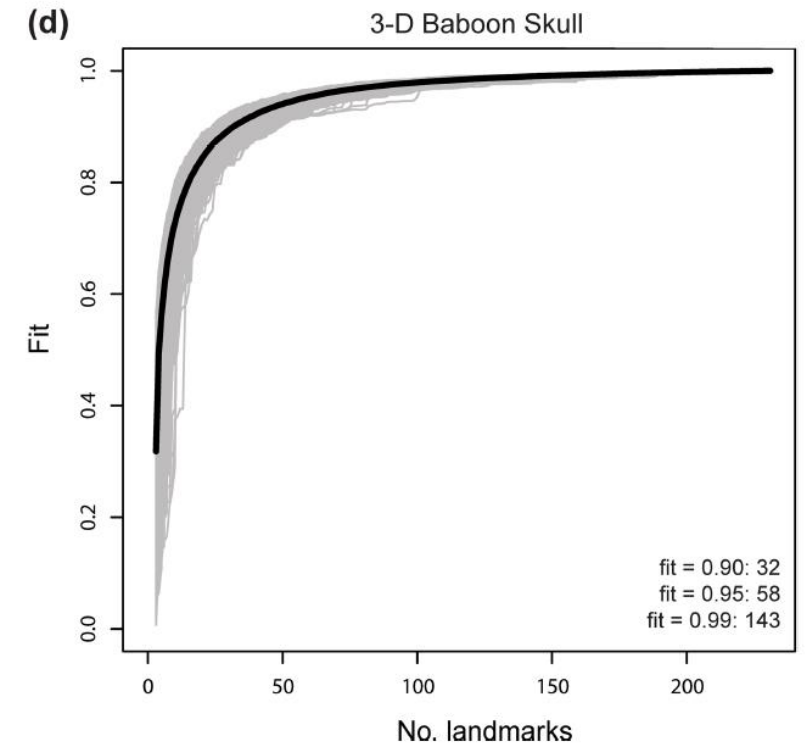
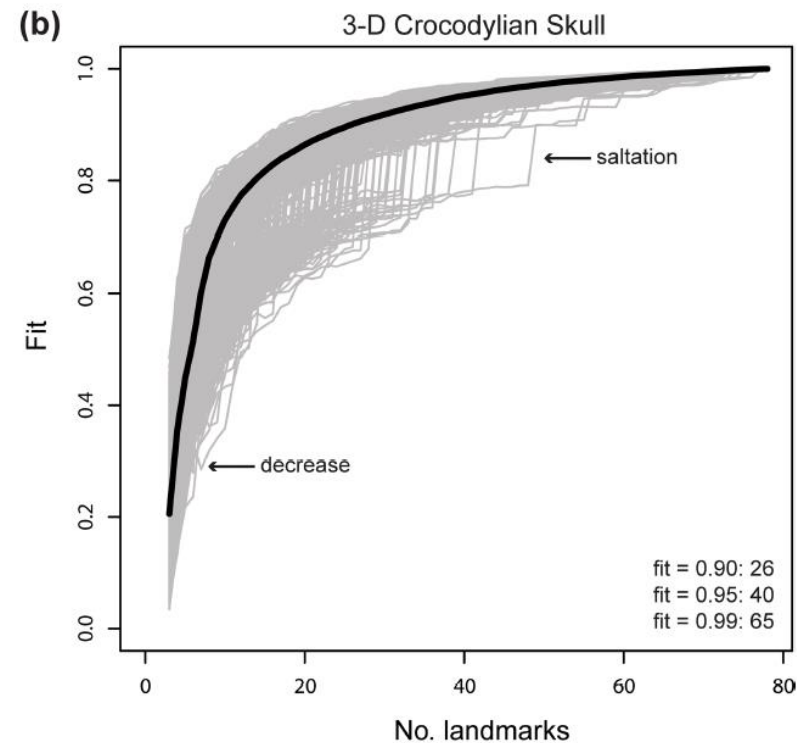
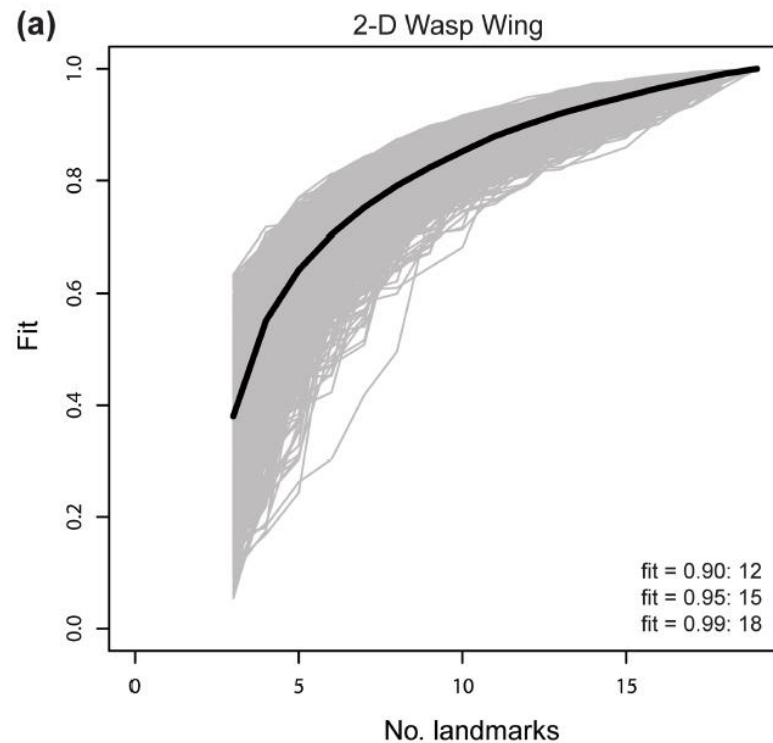
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Limitations of traditional landmarks

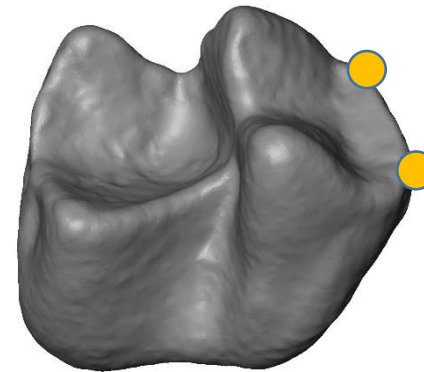
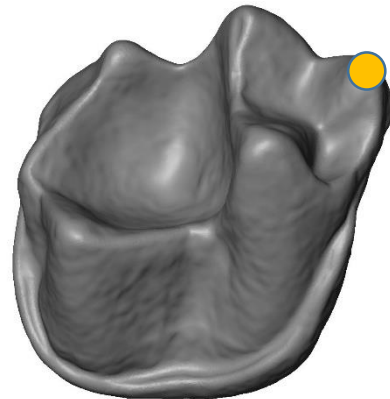
- 1) Time consuming for richly corresponding shapes
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Limitations of traditional landmarks

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

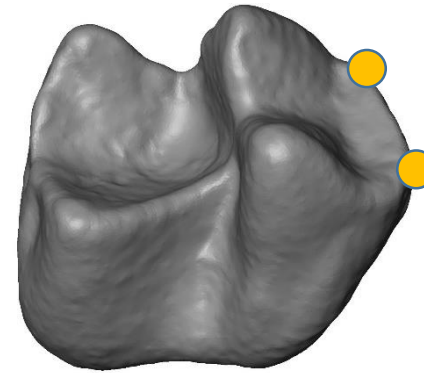
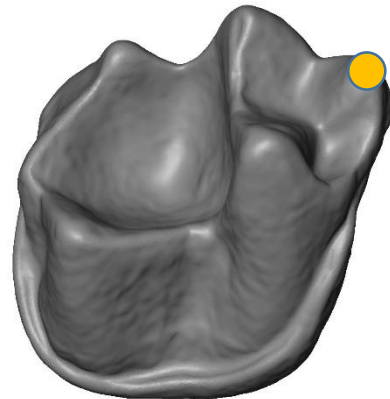
“As a general rule, landmarks should be chosen so you can quantify any differences that you can see” (Zelditch et al., 2004)



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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

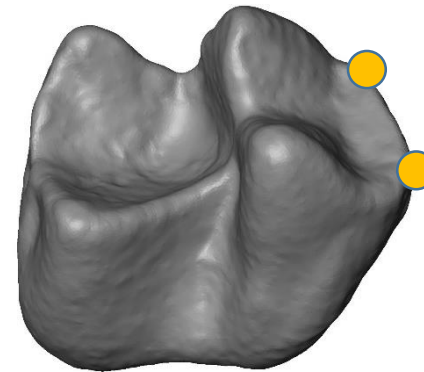
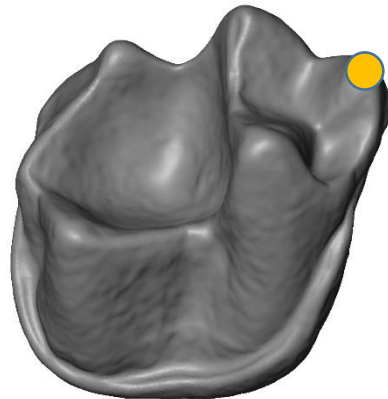


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Limitations of traditional landmarks

4) Cannot be used for “topology” changes

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

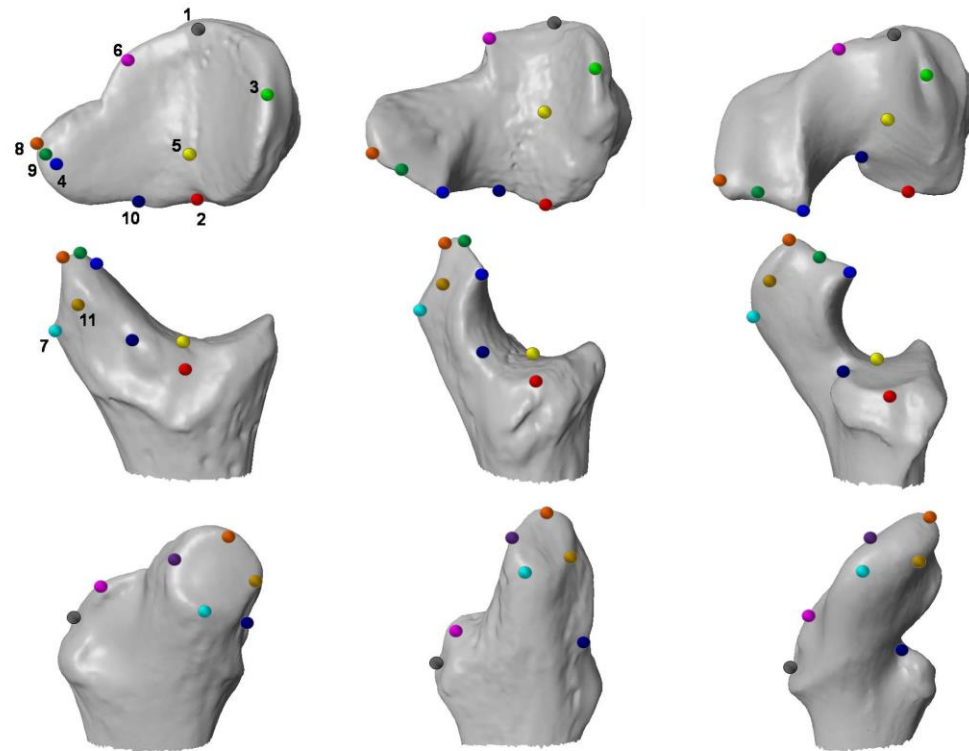


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Limitations of traditional landmarks

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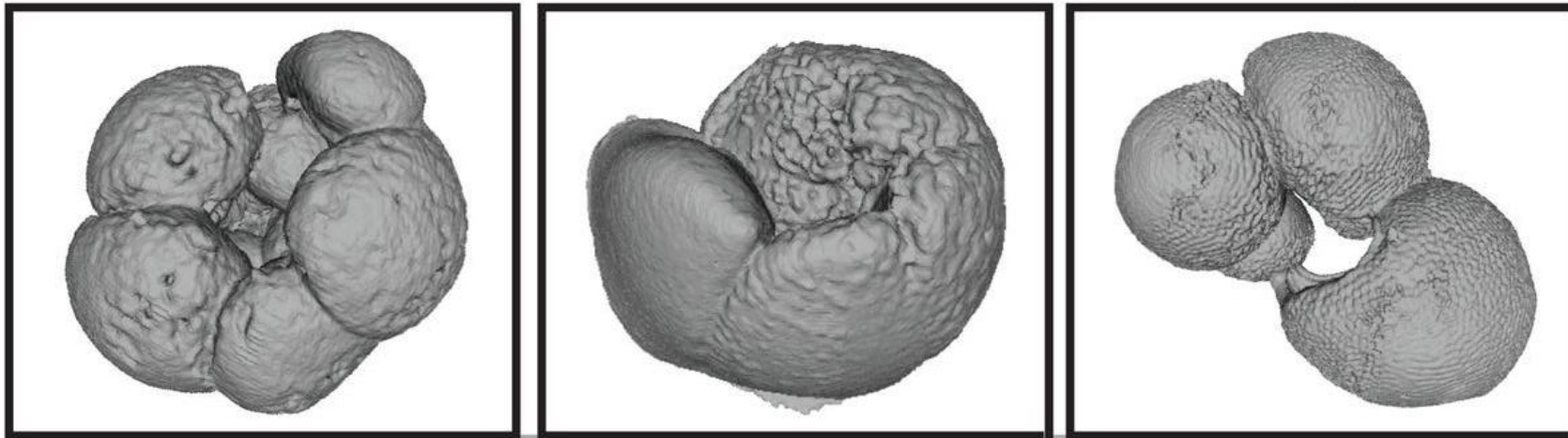
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Limitations of traditional landmarks

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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”

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.



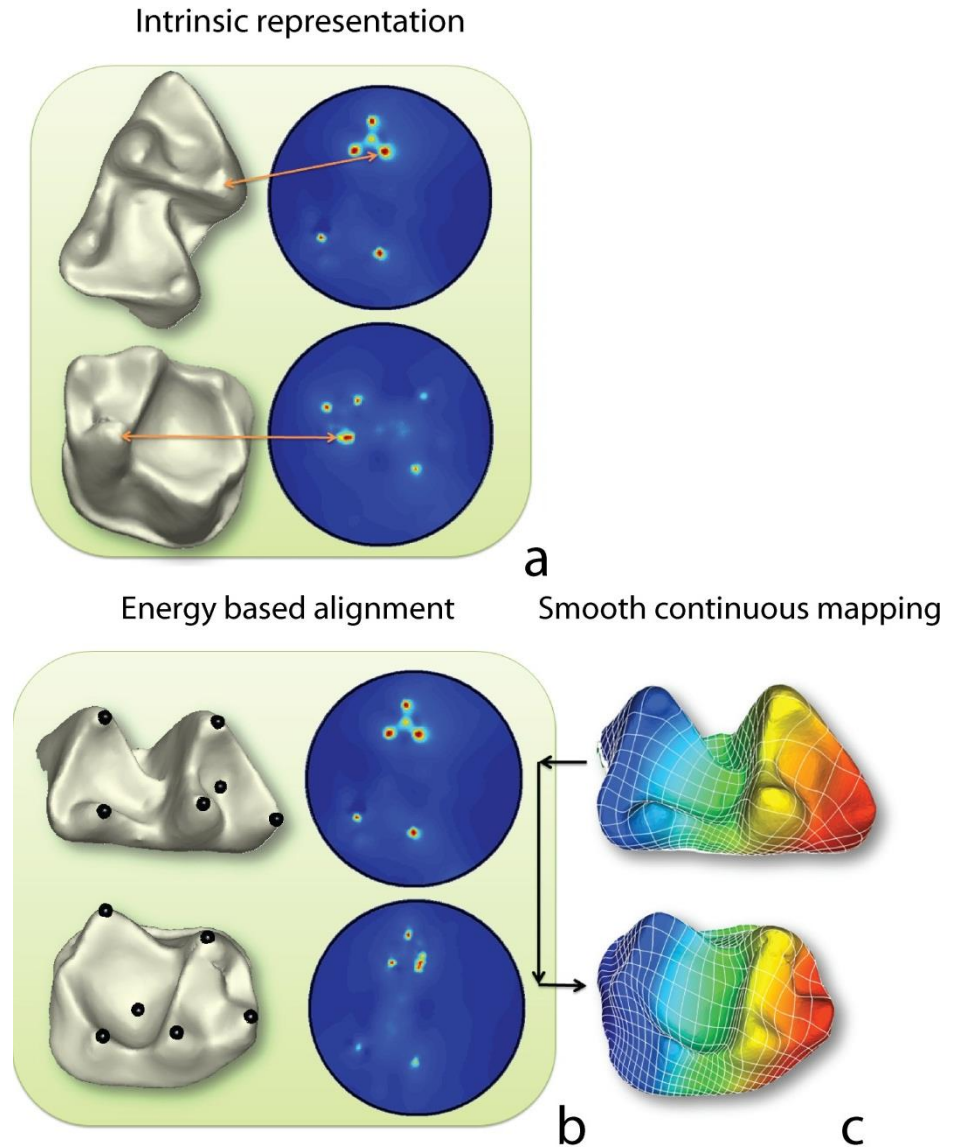
Initial Progress

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.



Results

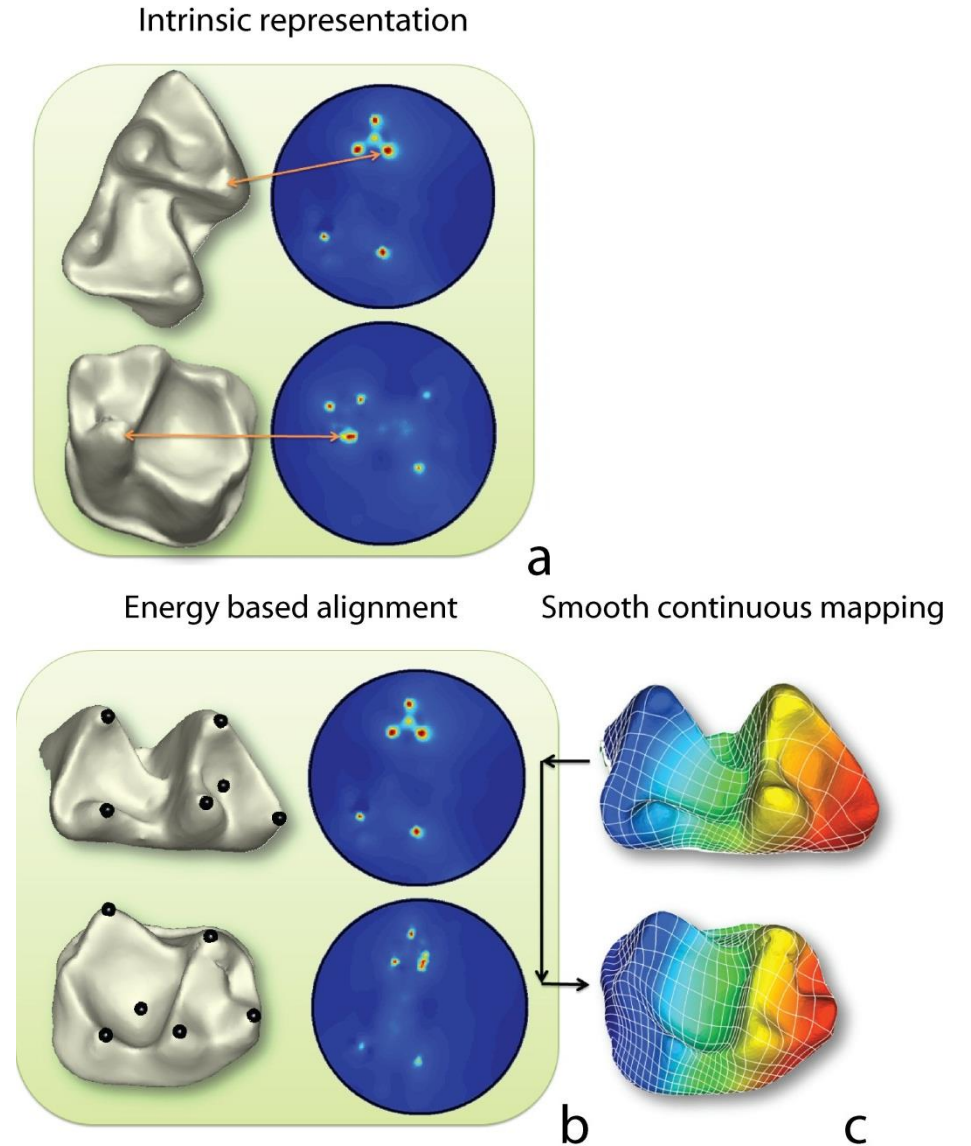
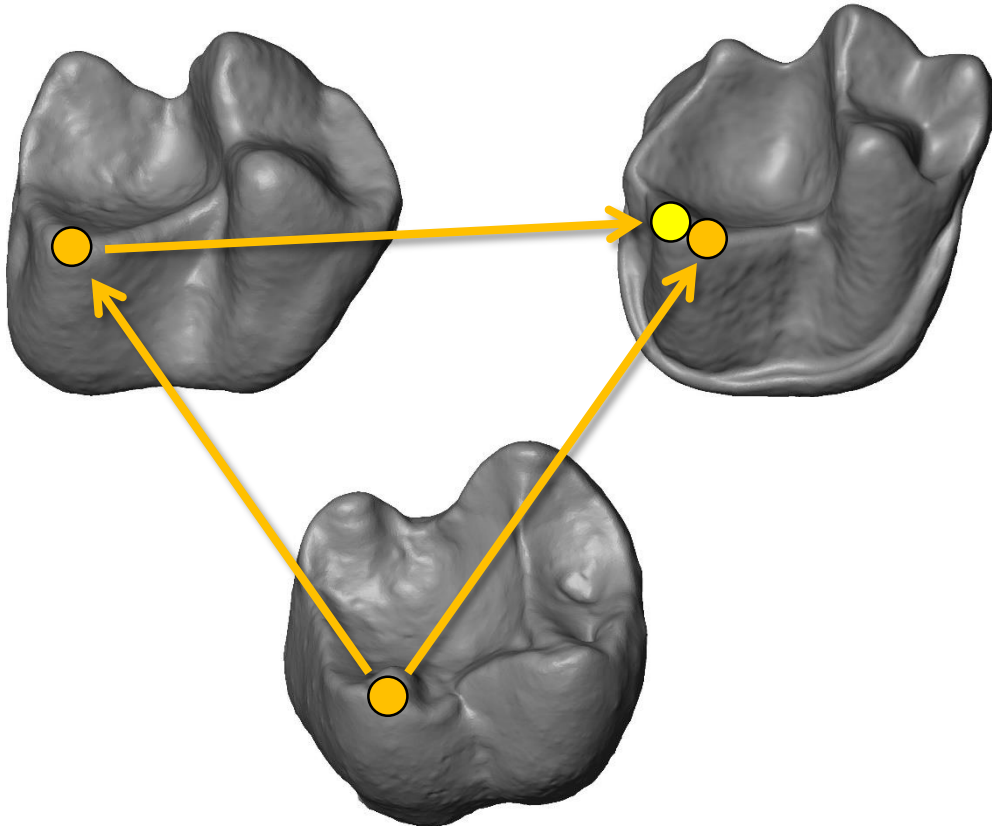
Classification success (mean % correct per genus)

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

Initial Progress

Limitations

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



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>

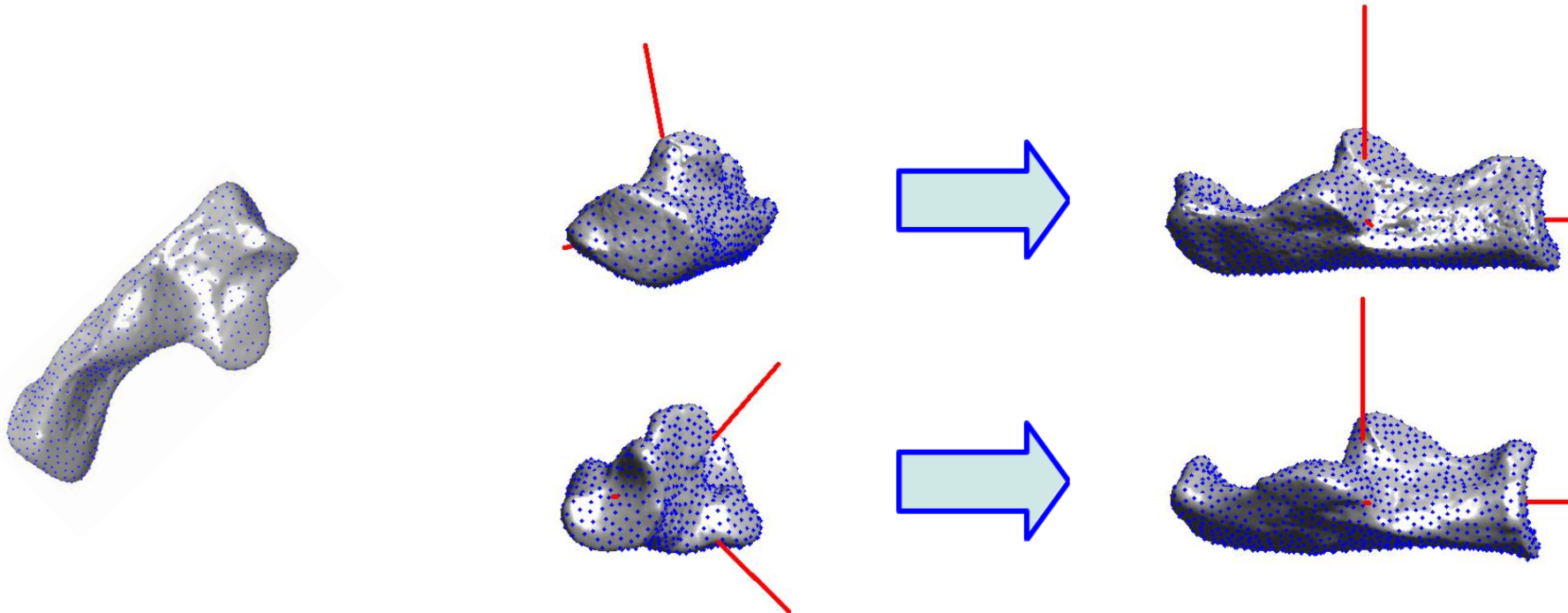
Applications (e.g):

- 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

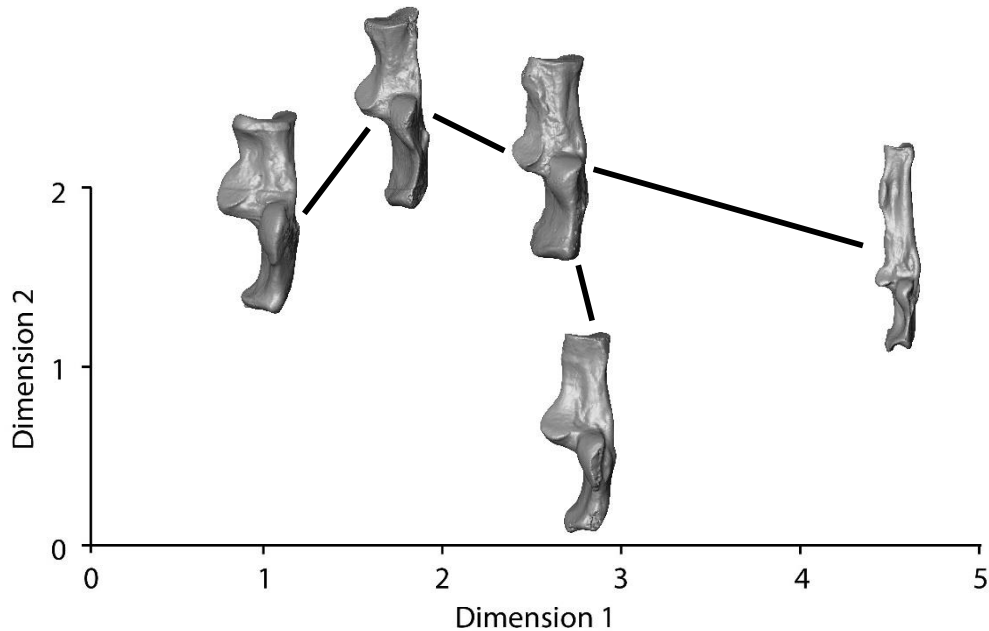
- Re-sample surface + size-standardize point cloud (Eldar et al. 1997)
- Compute principle axes with PCA
- Begin “alignment search”
 - Principle axes (8 possibilities)
 - Iterative closest points: Compute euclidean motions that minimize procrustes distance (PCD) (Besl & McKay 1992)













Steps to the method

Alignment refinement

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

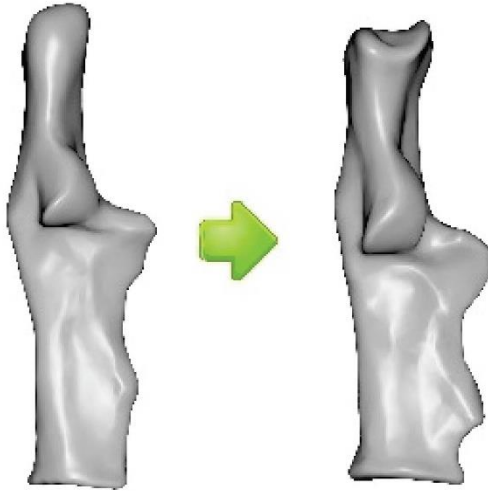


PCD matrix

					
	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

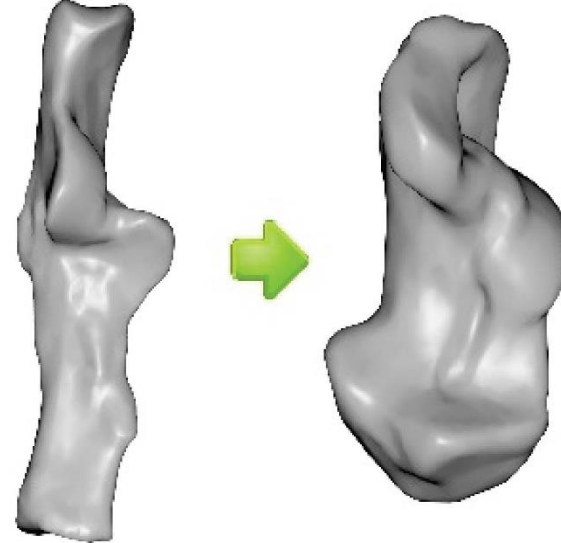
Purpose of MST & Propagation

Similar shapes align well



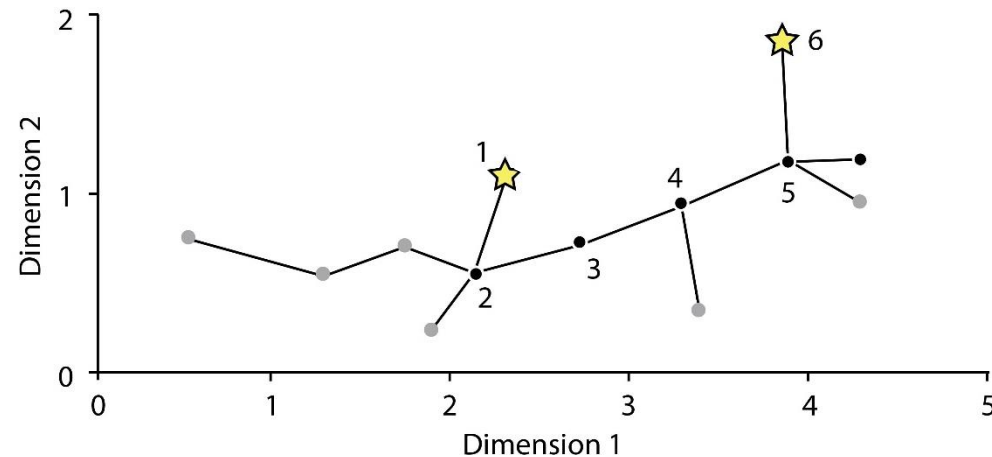
PCD = 0.1

Dissimilar shapes may align incorrectly



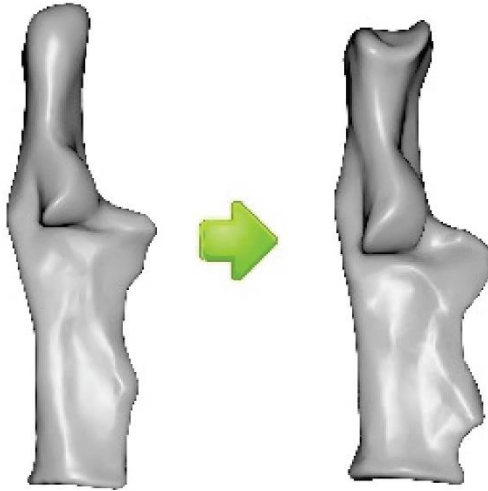
PCD = 0.7

All Procrustes distances used to construct initial minimum spanning tree



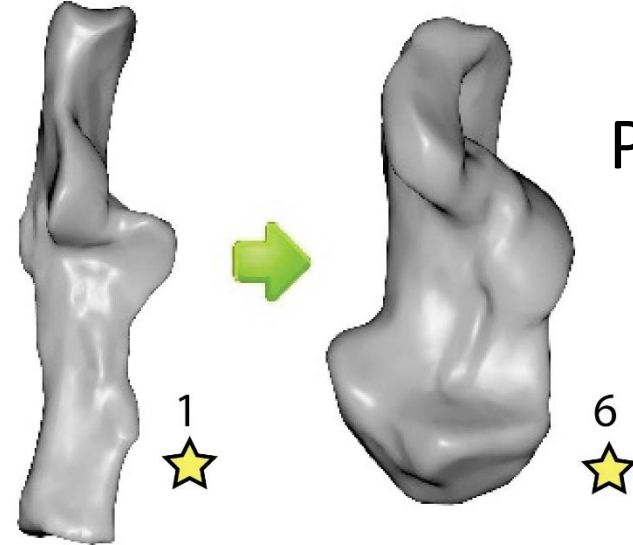
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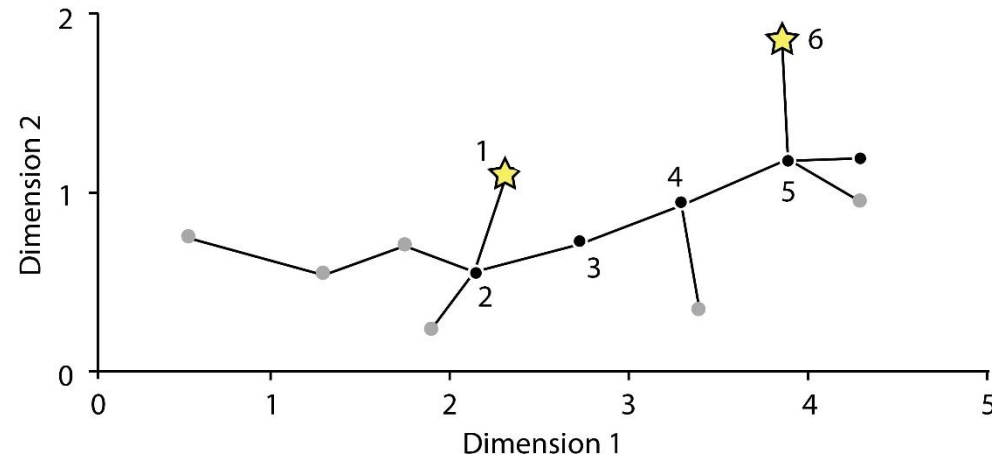
PCD = 0.1

Dissimilar shapes may align incorrectly



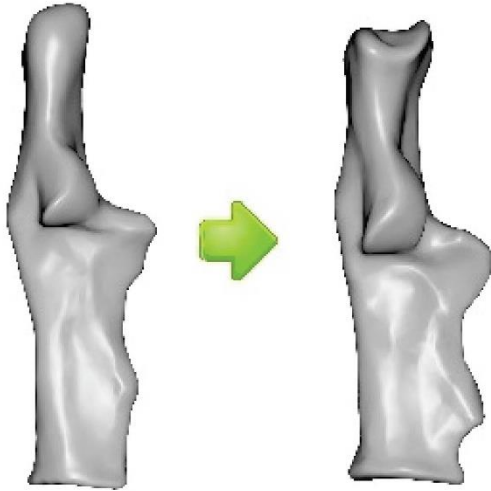
PCD = 0.7

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



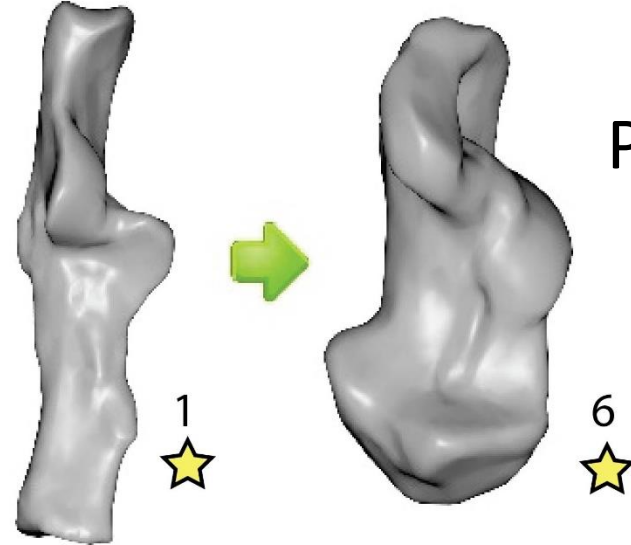
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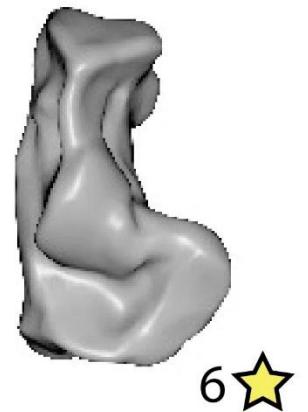
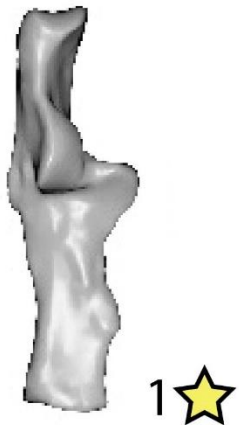
PCD = 0.1

Dissimilar shapes may align incorrectly

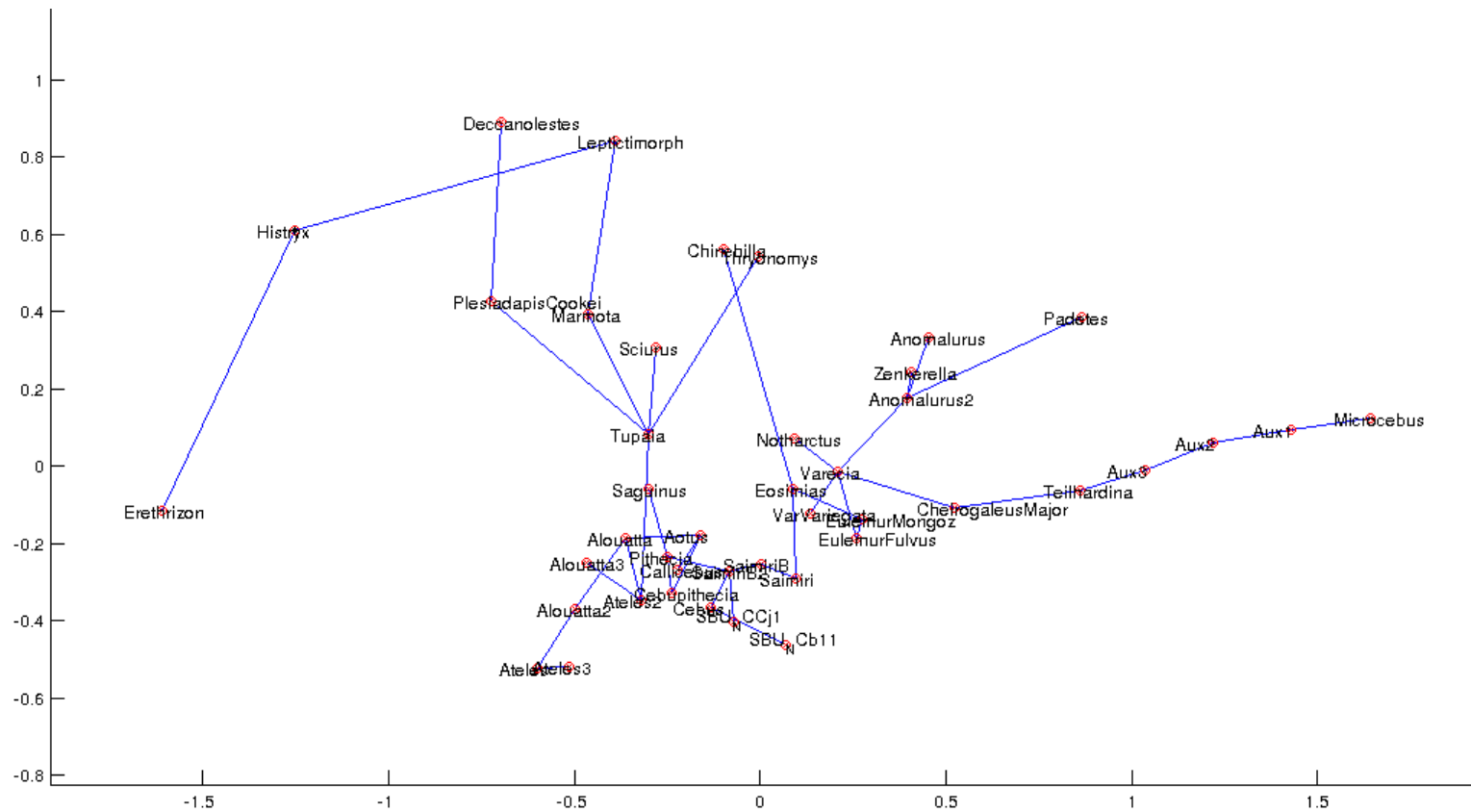


PCD = 0.7

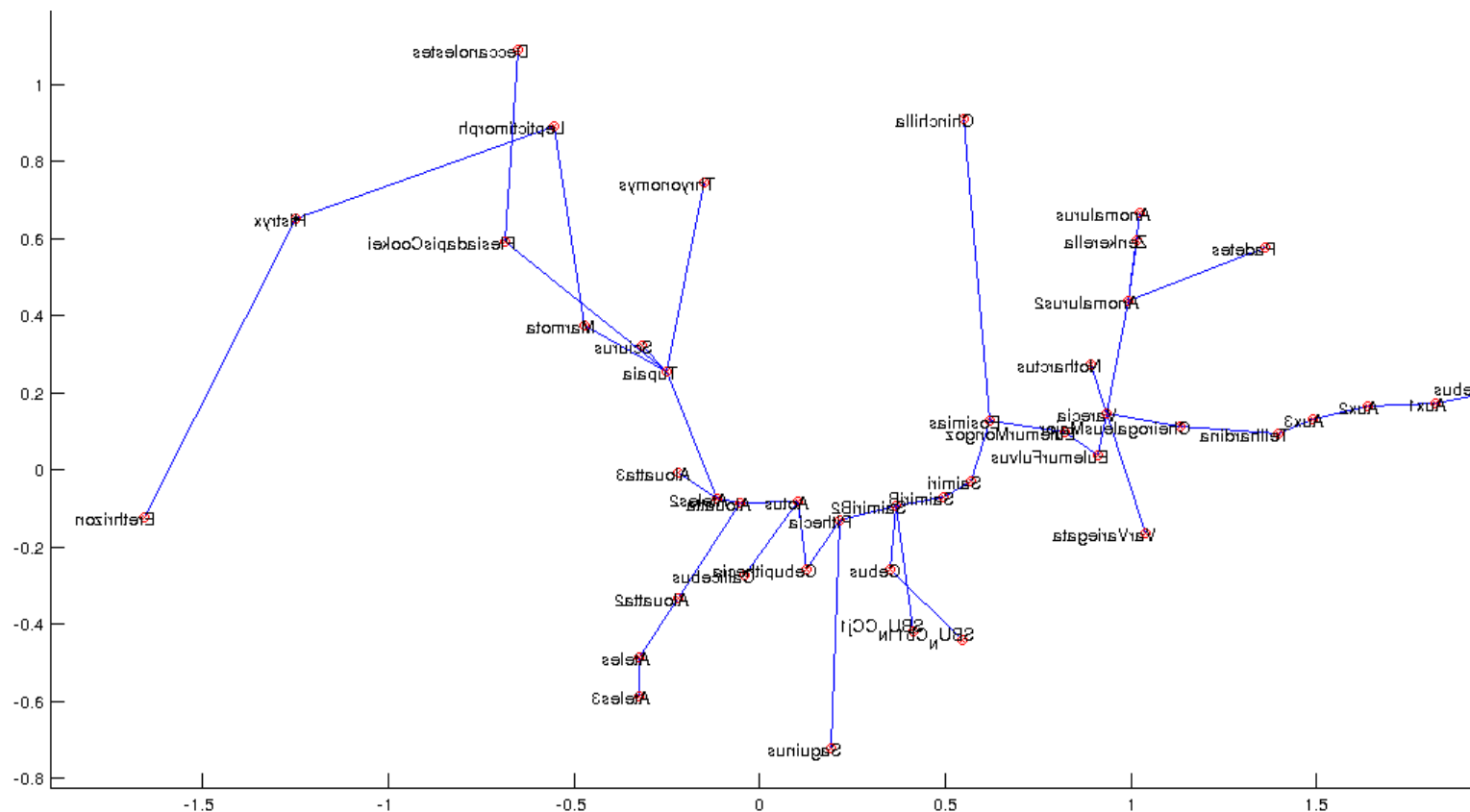
The MST path can be used to find correct alignments, and recompute distances



MST w initial correspondences

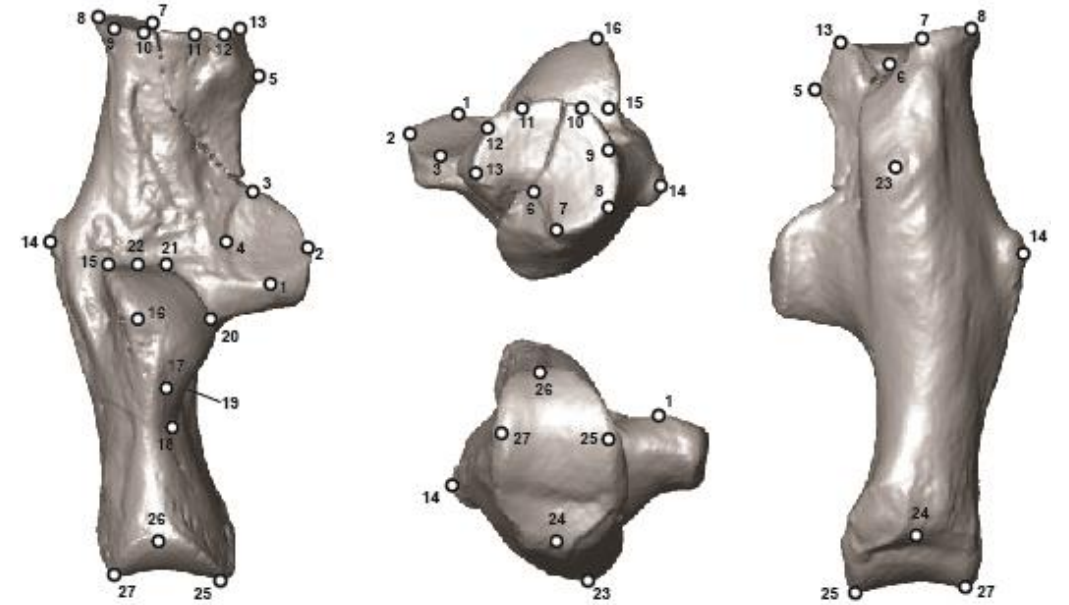


MST w transitive correspondences



Comparison to researcher-based data set

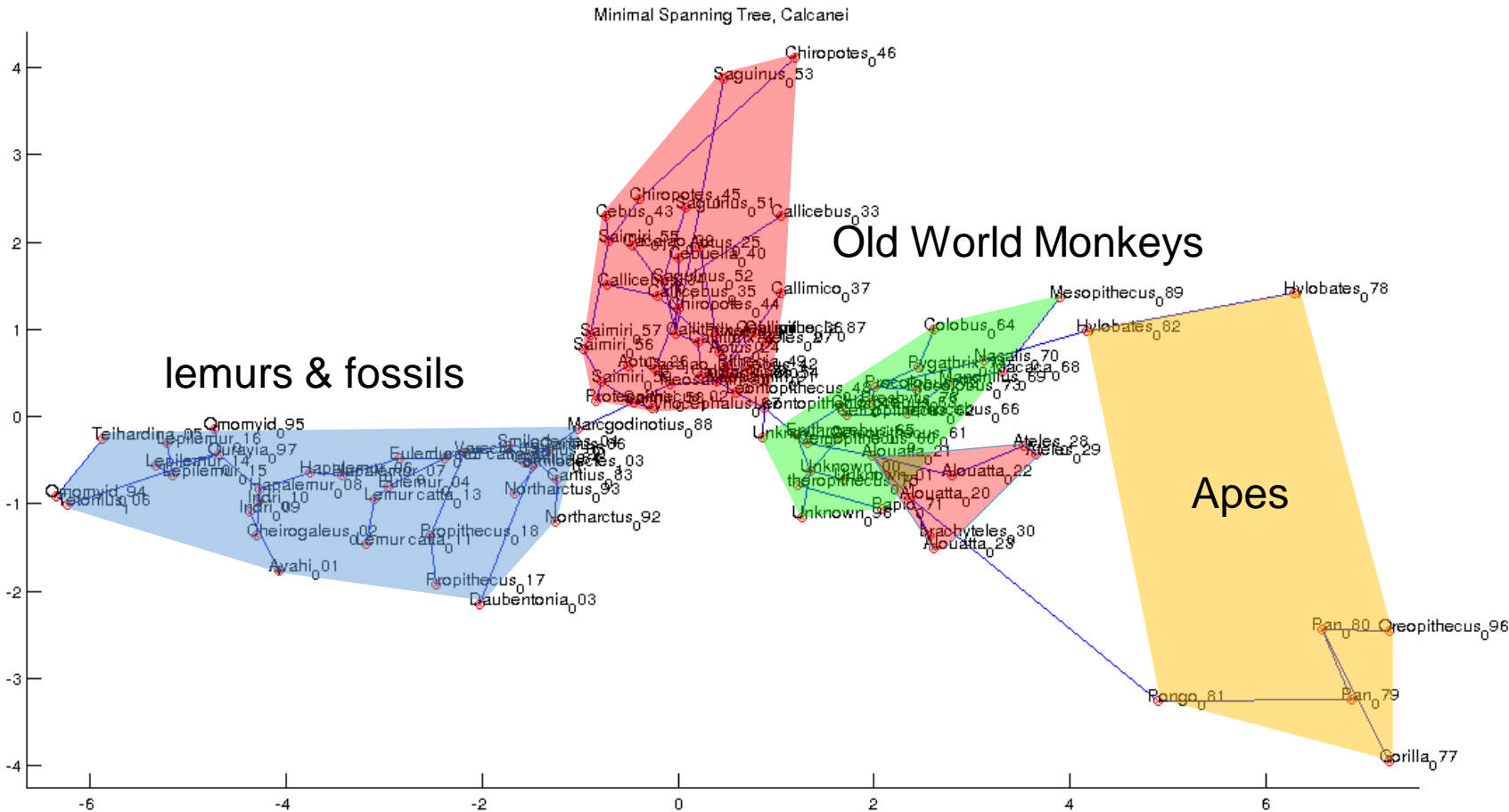
- Sample - 106 calcanei
- Data points
 - Observer (27 landmarks)
 - Algorithm (1,024 points)
- Software
 - *Morphologika2.5*
- Both datasets analyzed identically



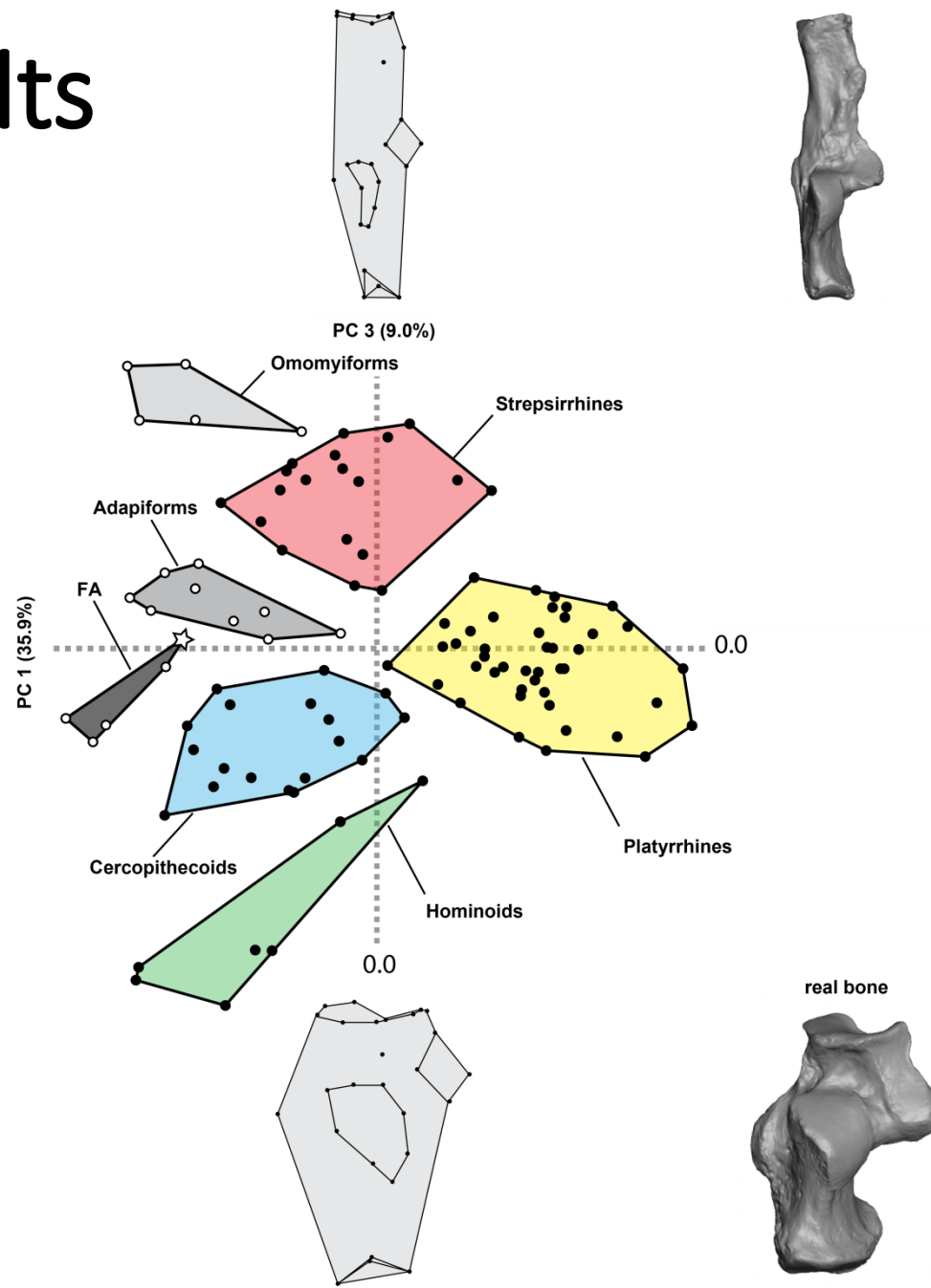
From *Gladman et al. (2013)*

Results

South American monkeys



Results

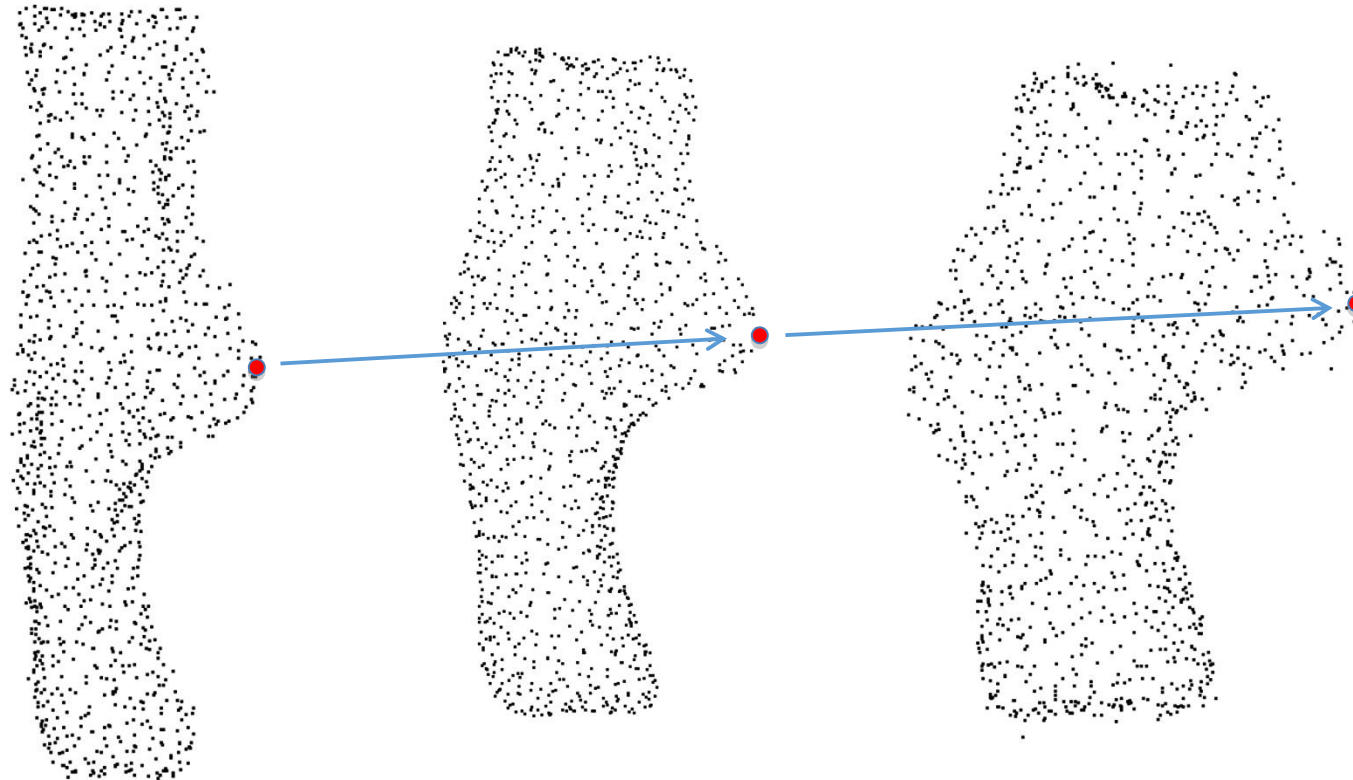


Other stuff...

Some other properties/limitations

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

What we want (?)

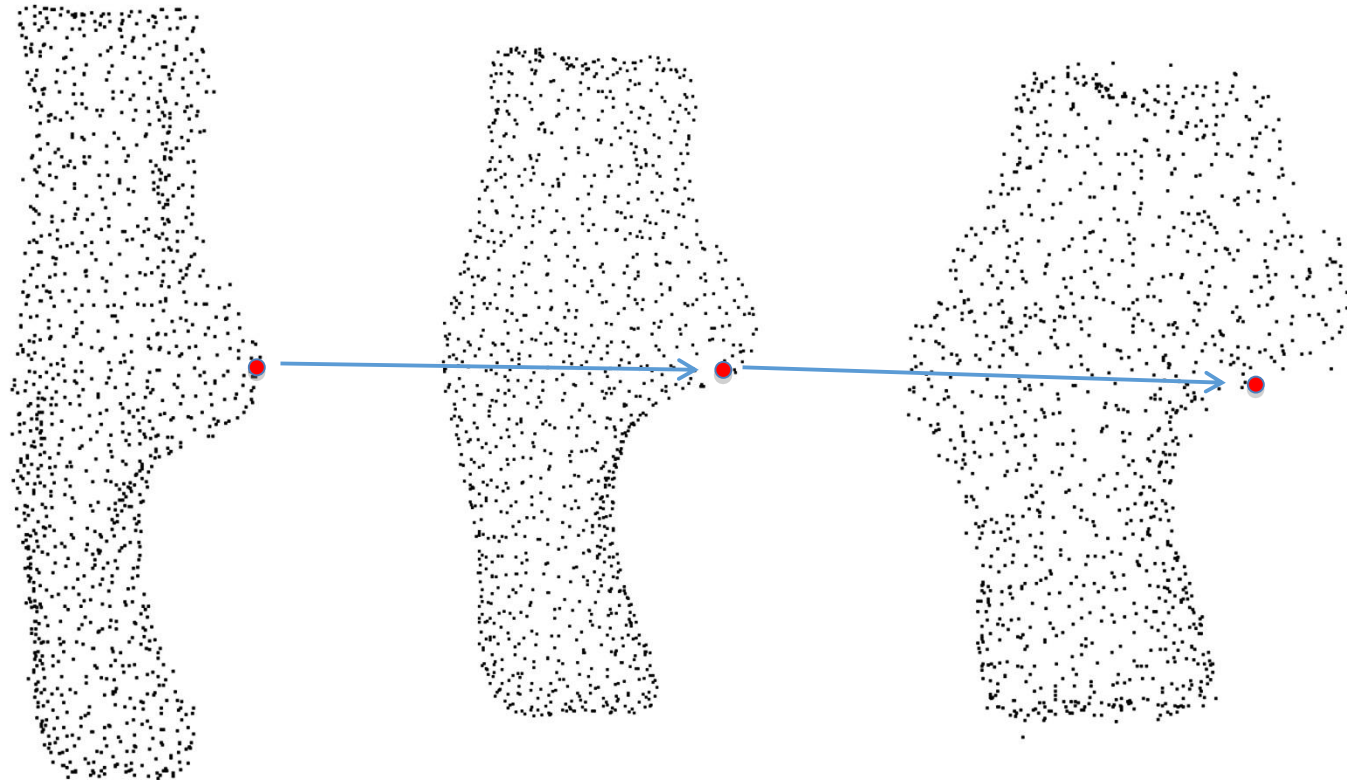


Other stuff...

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)

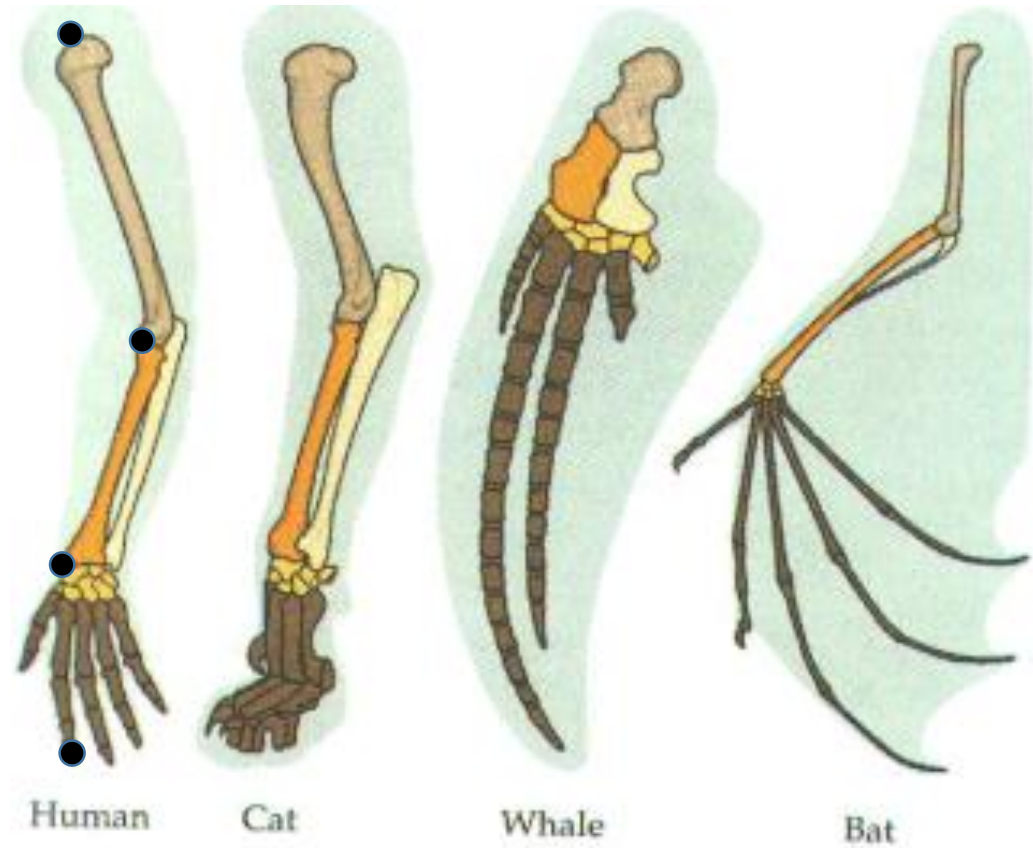
“biological homology refers to unitary structures; not to the infinitesimal coordinate locations on structures that can be defined under the concept of geometric homology” (MacLeod, 2001)

Homology

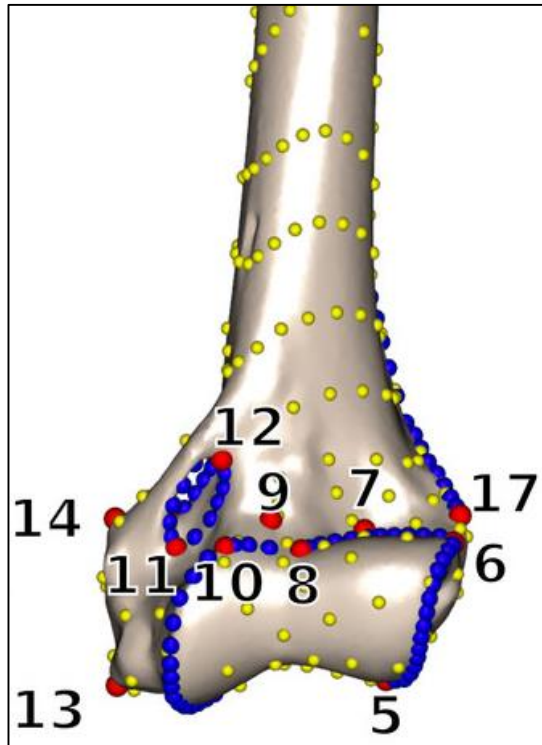
- Kinds of Homology
 - Transformational (aka 'genealogical' or 'Darwinian')
 - Serial (homologous by developmental duplication)
 - Operational (hypothesis for the purpose of communication or measurement)
 - Taxic (variation in transformational homologous features)

Homology

Biological homology & geometric homology converge nicely in a skull



Homology of facet boundaries as 'type 1'

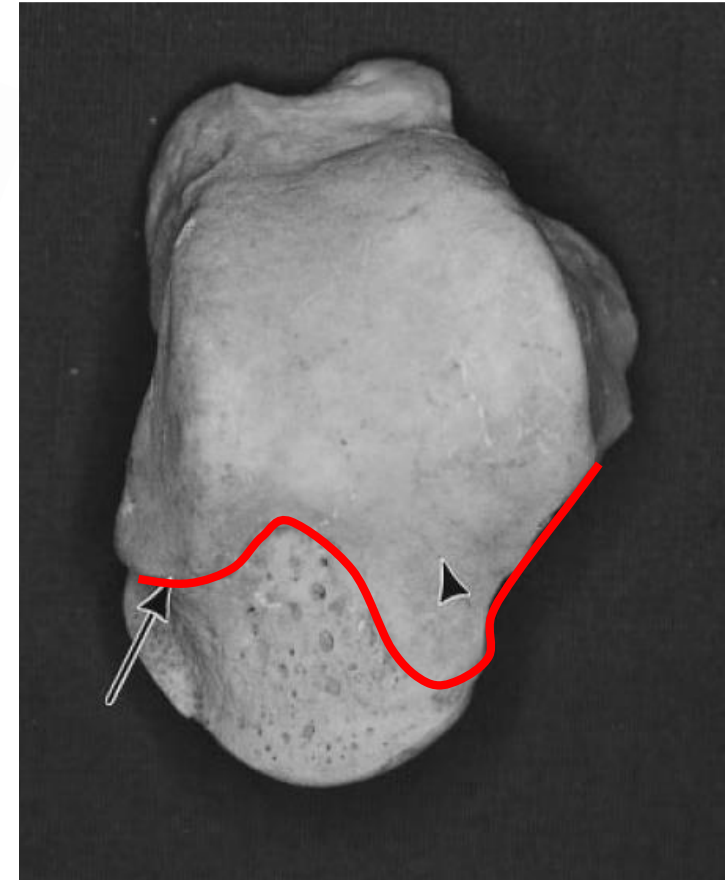


Left humerus, distal end,
anterior view

Bonn-Divett et al. (2019)

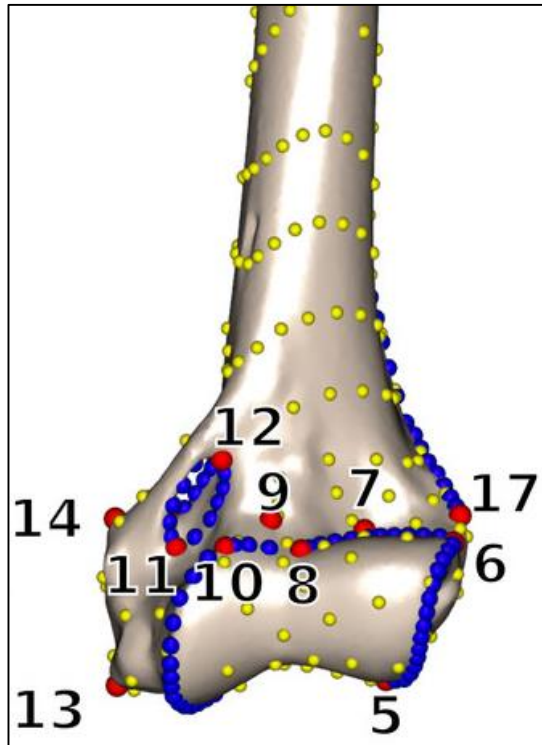


Left talus, dorsal view

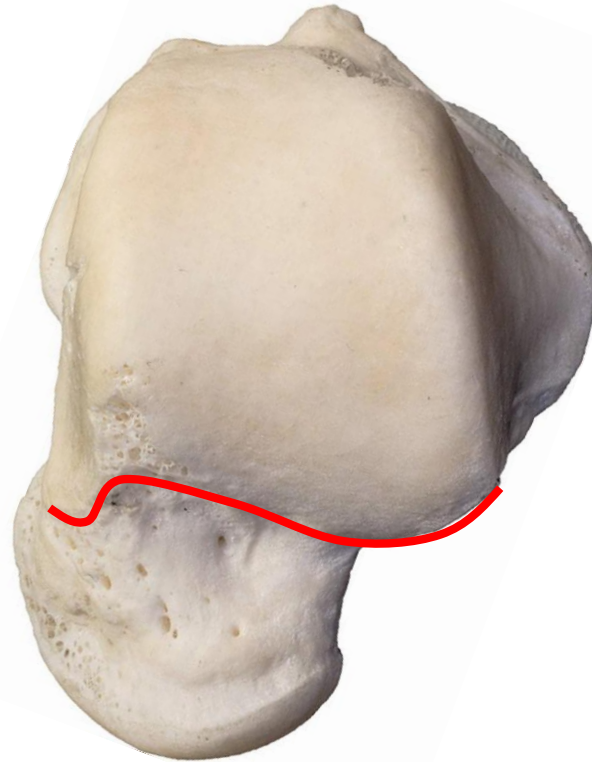


Barnet (1954)

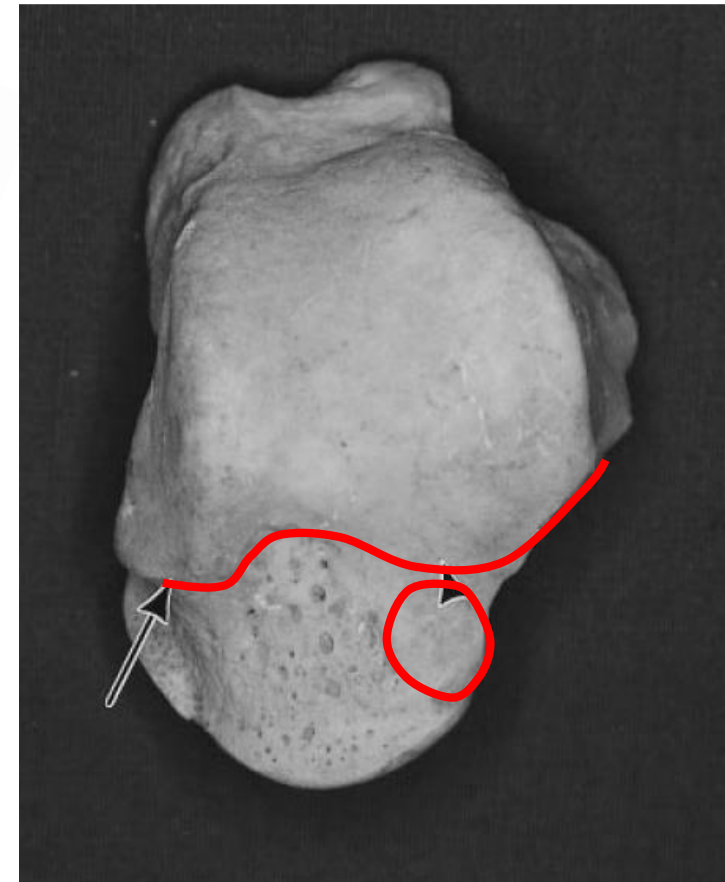
Homology of facet boundaries as 'Type 1'



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



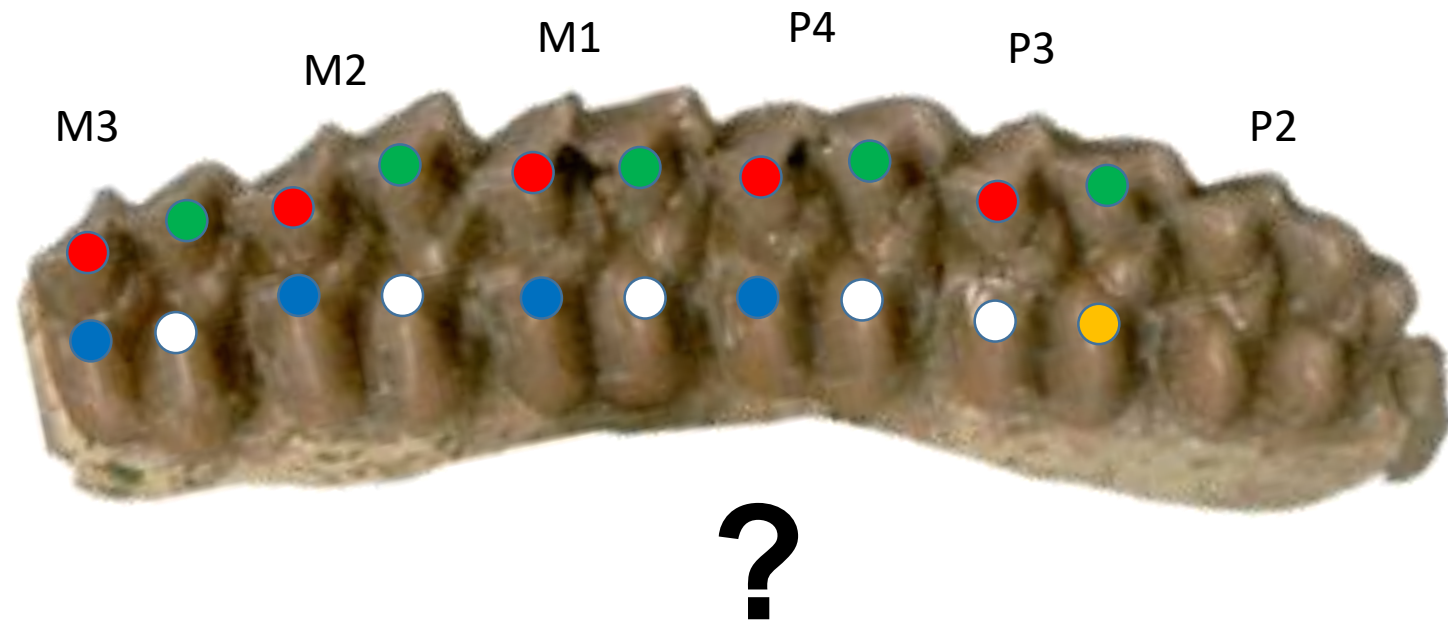
Left talus, dorsal view



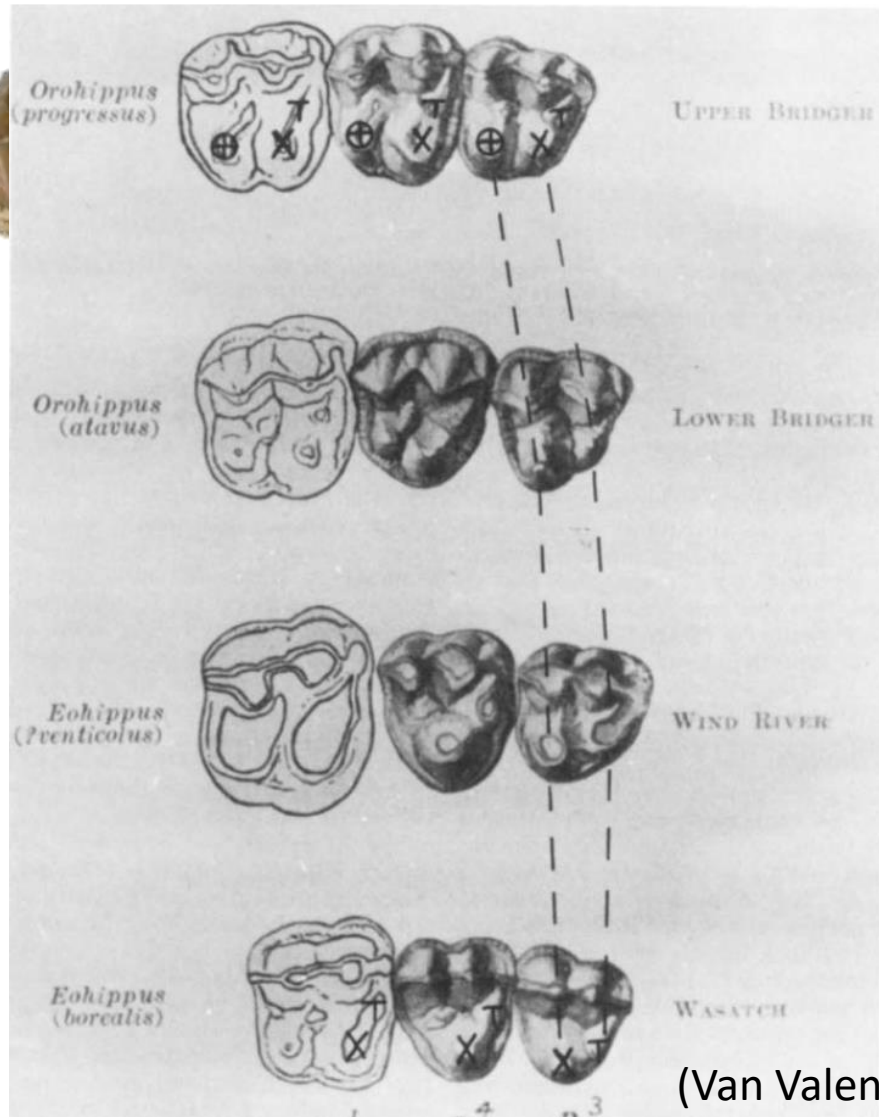
Barnet (1954)

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Homology of tooth cusps



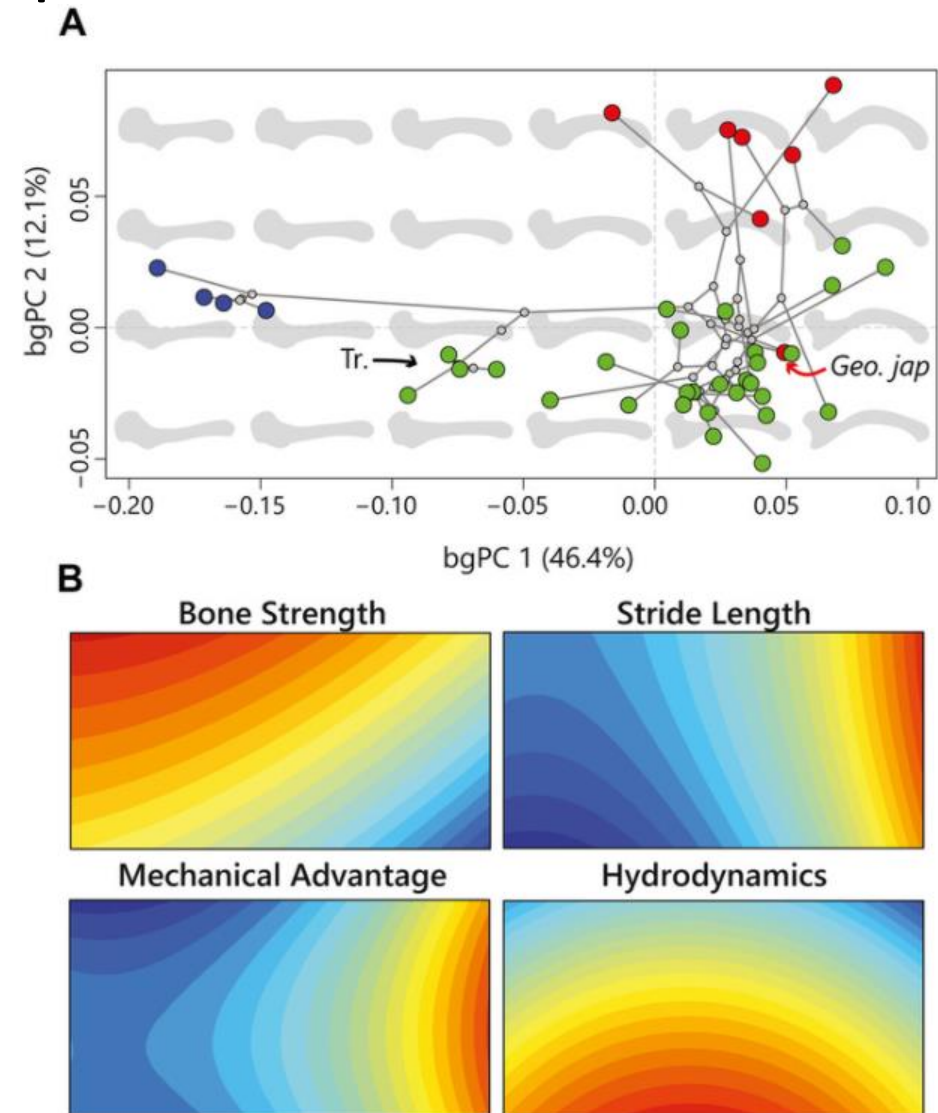
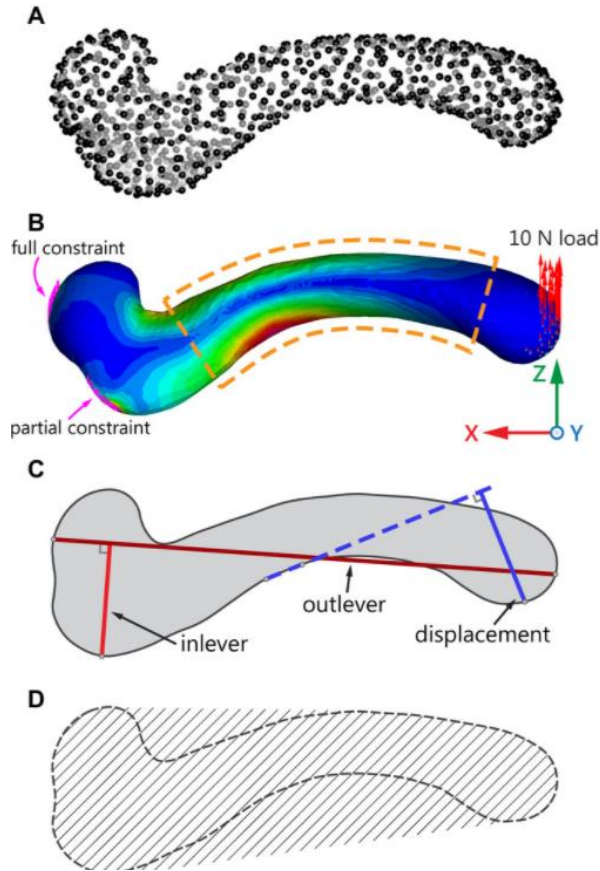
Homology of tooth cusps



(Van Valen, 1982)

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

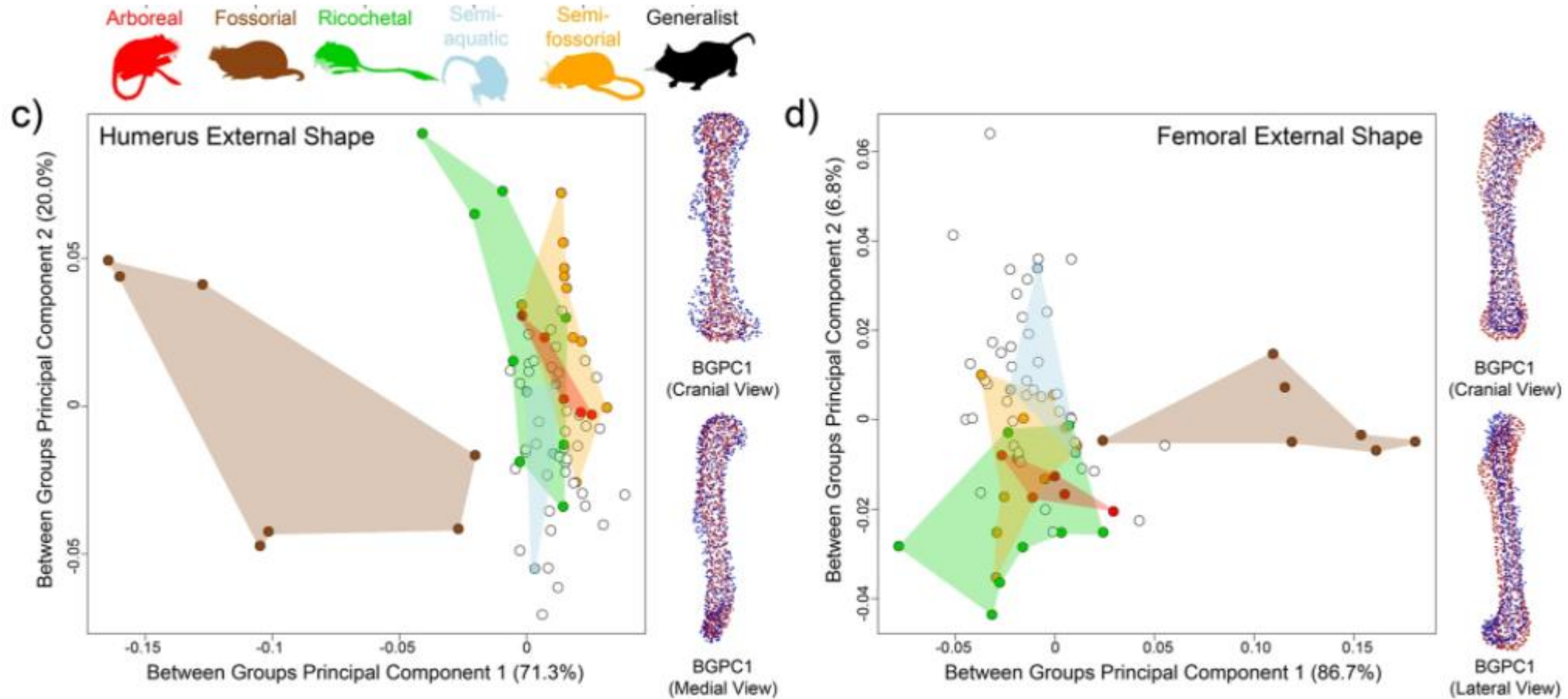
Inspiring applications



Dickson et al. (2019) *Evolution*

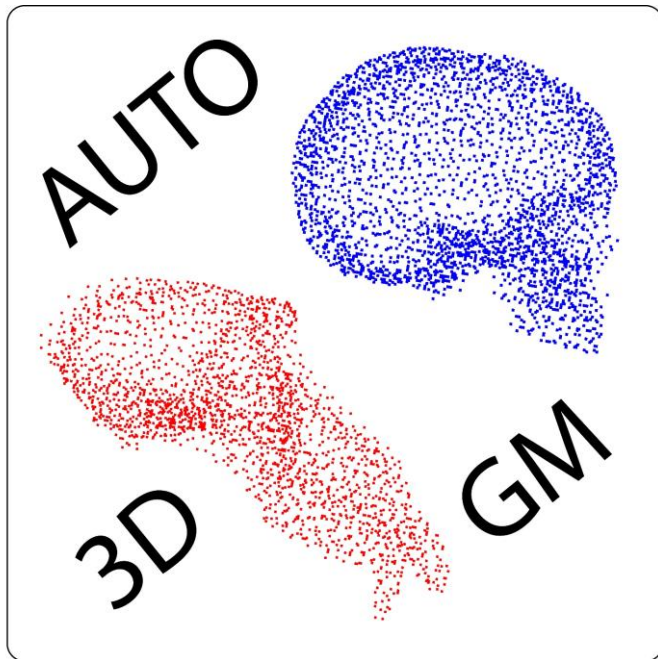
<https://doi.org/10.1111/evo.13747>

Inspiring applications

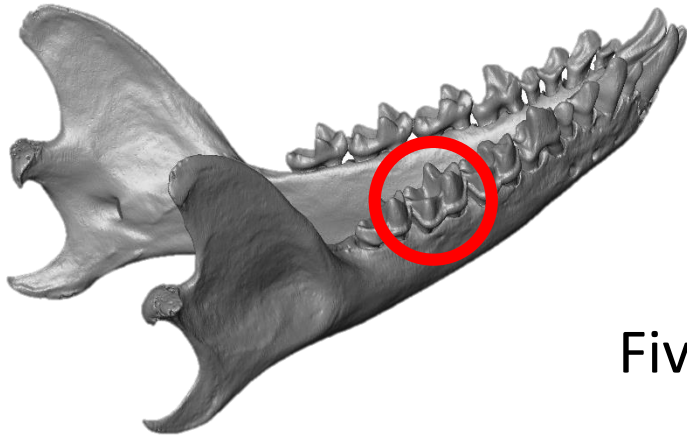


Hedrick et al. (2020) *Sci Rep* <https://doi.org/10.1038/s41598-019-57144-w>

Slicer auto3dgm

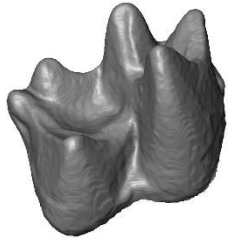


- Available from Slicer Extension manager
 - Bundled with SlicerMorph extension
 - Also available separately
- Documentation at this website:
<https://toothandclaw.github.io/>
- Other implementations of auto3dgm also available
 - R, matlab, python



Today's sample

Five living mammal groups: second lower molars



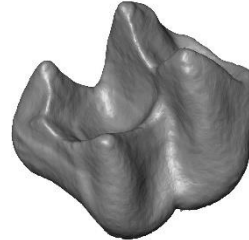
x 3

treeshrew



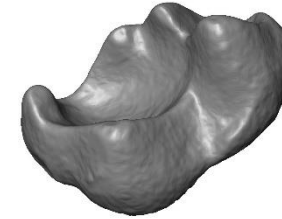
x 3

tarsier



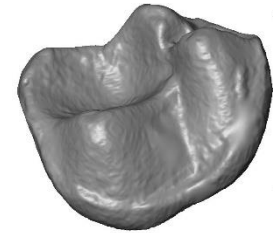
x 3

bush baby



x 3

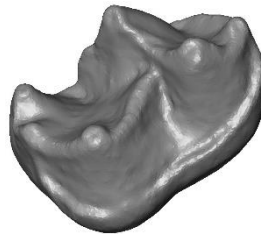
lemur



x 3

mouse lemur

Five fossils...



Questions

Are the living groups distinct?

Do the fossils appear to be attributable to different living clades?