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Supplementary Materials for

Increasing morphological disparity and decreasing optimality for jaw speed and strength during the radiation of jawed vertebrates

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This PDF file includes:

Figs. S1 to S12
Dataset S1
References

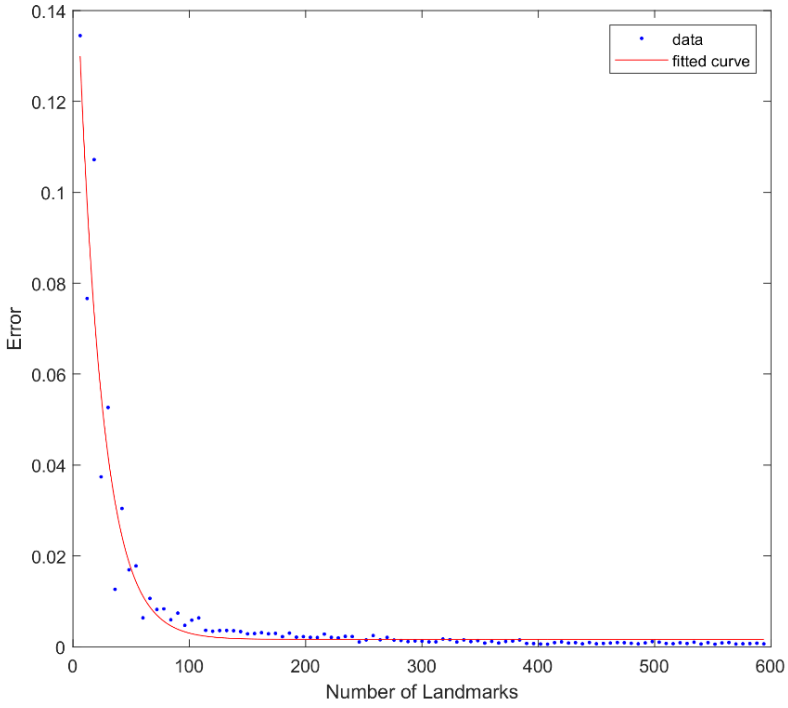


Fig S1: Landmark convergence test on *Acanthostega* outline. Optimal convergence is reached significantly before the chosen number, 600. 600 was chosen because it was the maximum possible number usable across all images, given varying image resolution, and the landmark number does not affect computation time significantly.

Morphospace

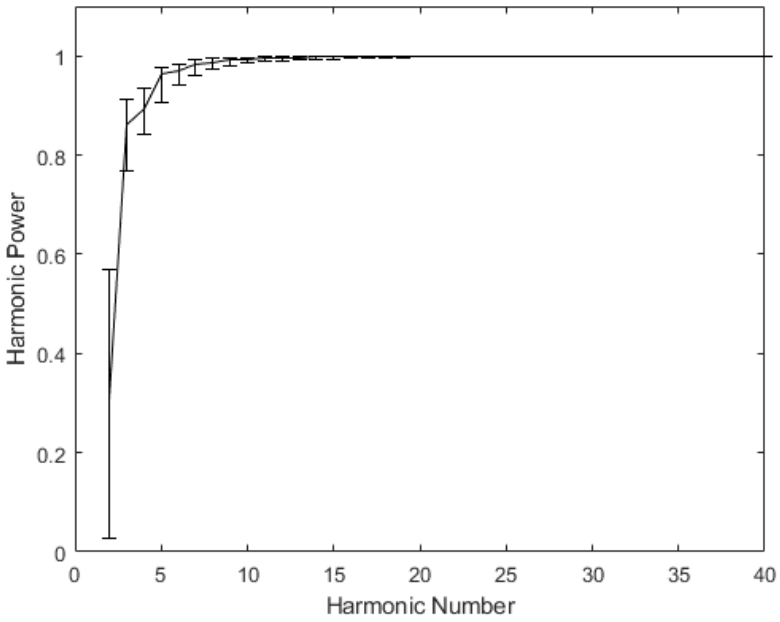


Fig S2: Harmonic power convergence across all taxa. Optimum number of harmonics was chosen as the point where the 5th percentile of taxa crosses the 0.99 power boundary (12 harmonics).

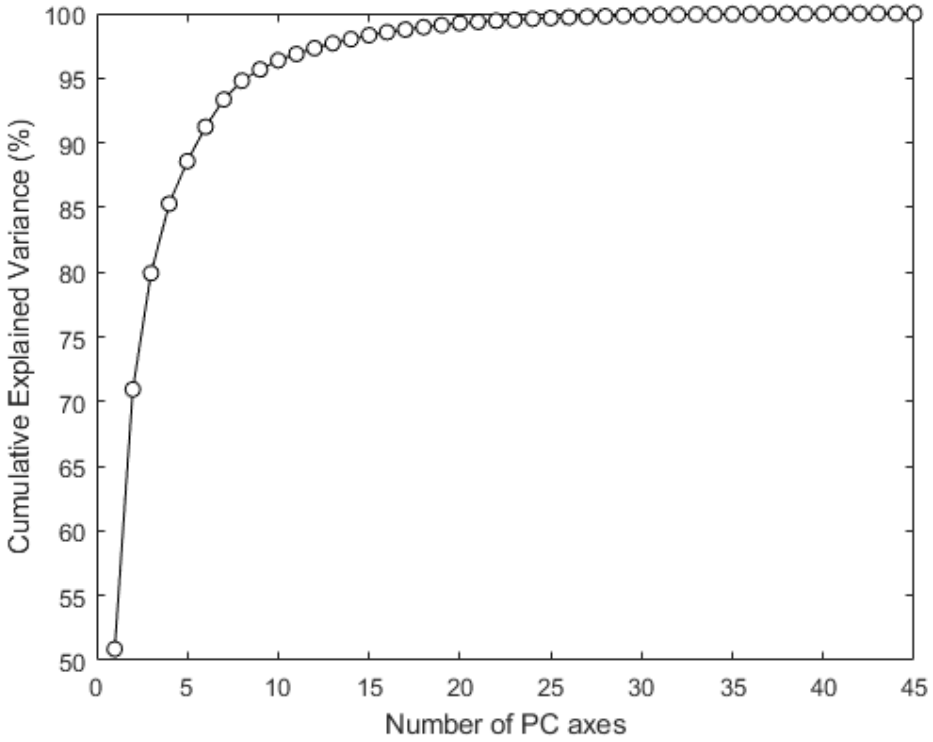
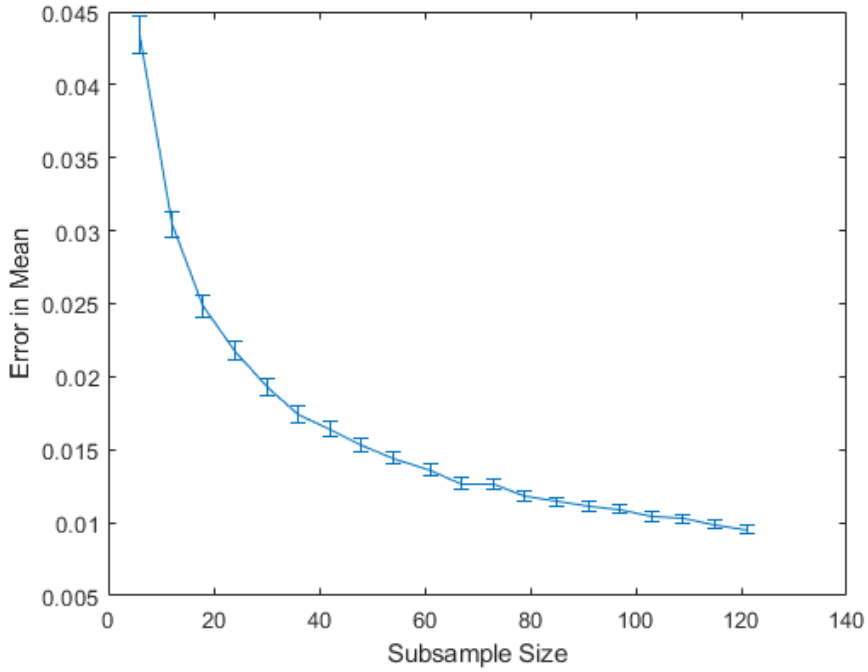


Fig S3: PCA Scree plot.



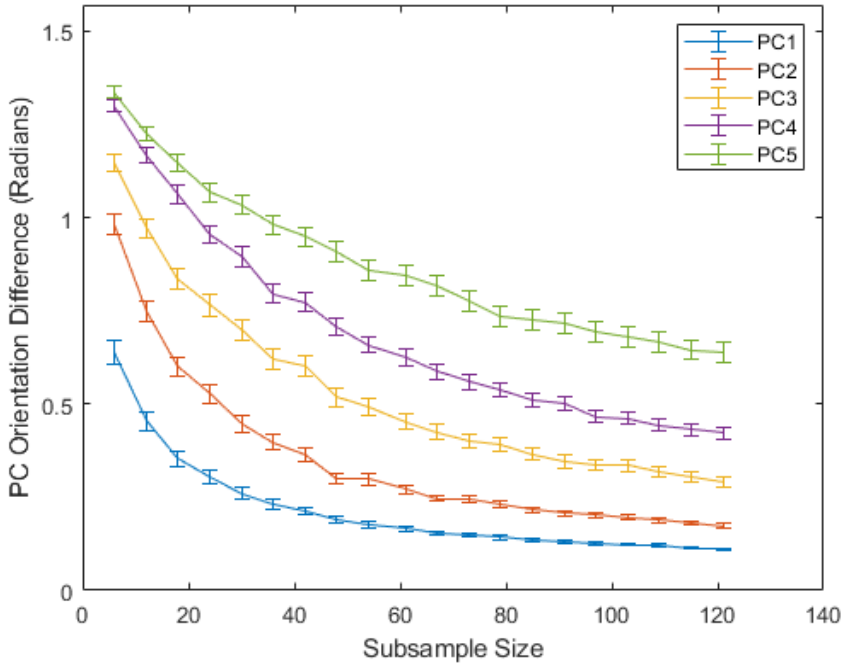


Fig S4: Sensitivity tests on theoretical morphospace at different sample sizes. Subsamples are built from bootstrapping the taxa and reperforming PCA. Top: Error in mean, Bottom: Error in orientation of the first 5 PC axes.

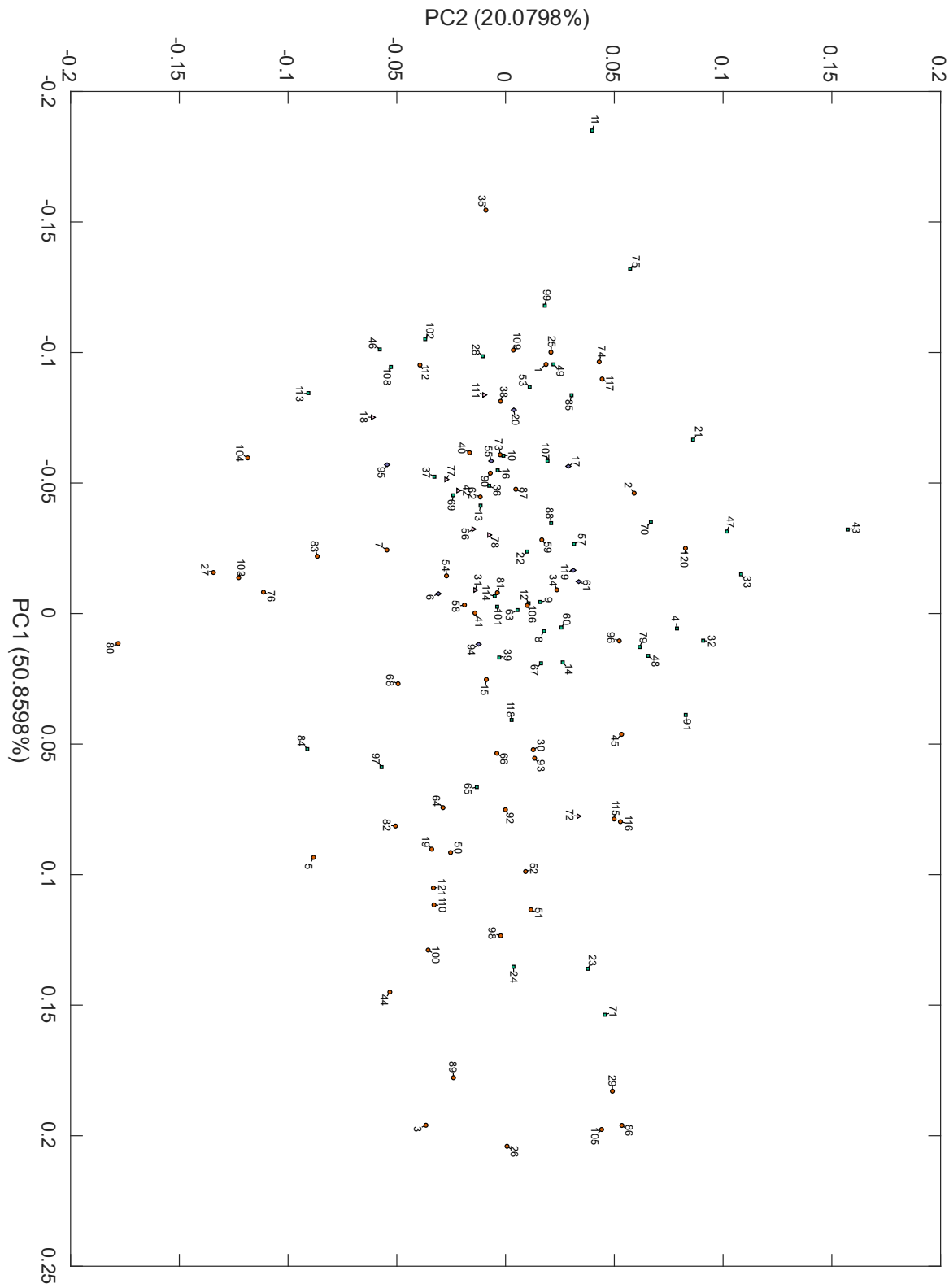


Fig S5: PC axes 1 and 2 with individual taxa labelled. Numbers represent taxon index (See Dataset S1A)

Functional Performance

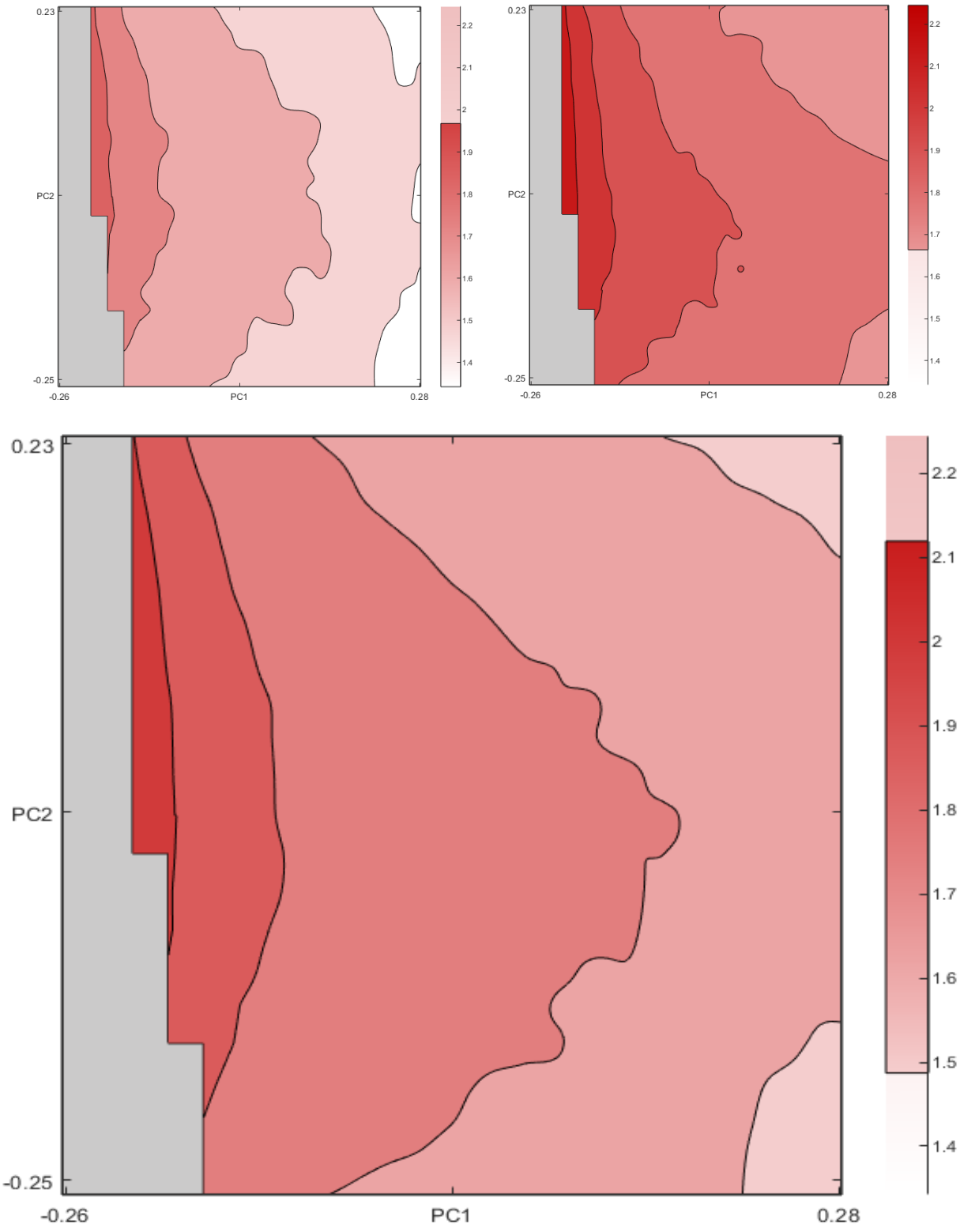


Fig S6: Rotational Efficiency (RE) surface plots. Top left: 5th percentile result of 1000 randomised inputs. Top right: 95th percentile result of 1000 randomised inputs. Bottom: mean result of 1000 randomised inputs.

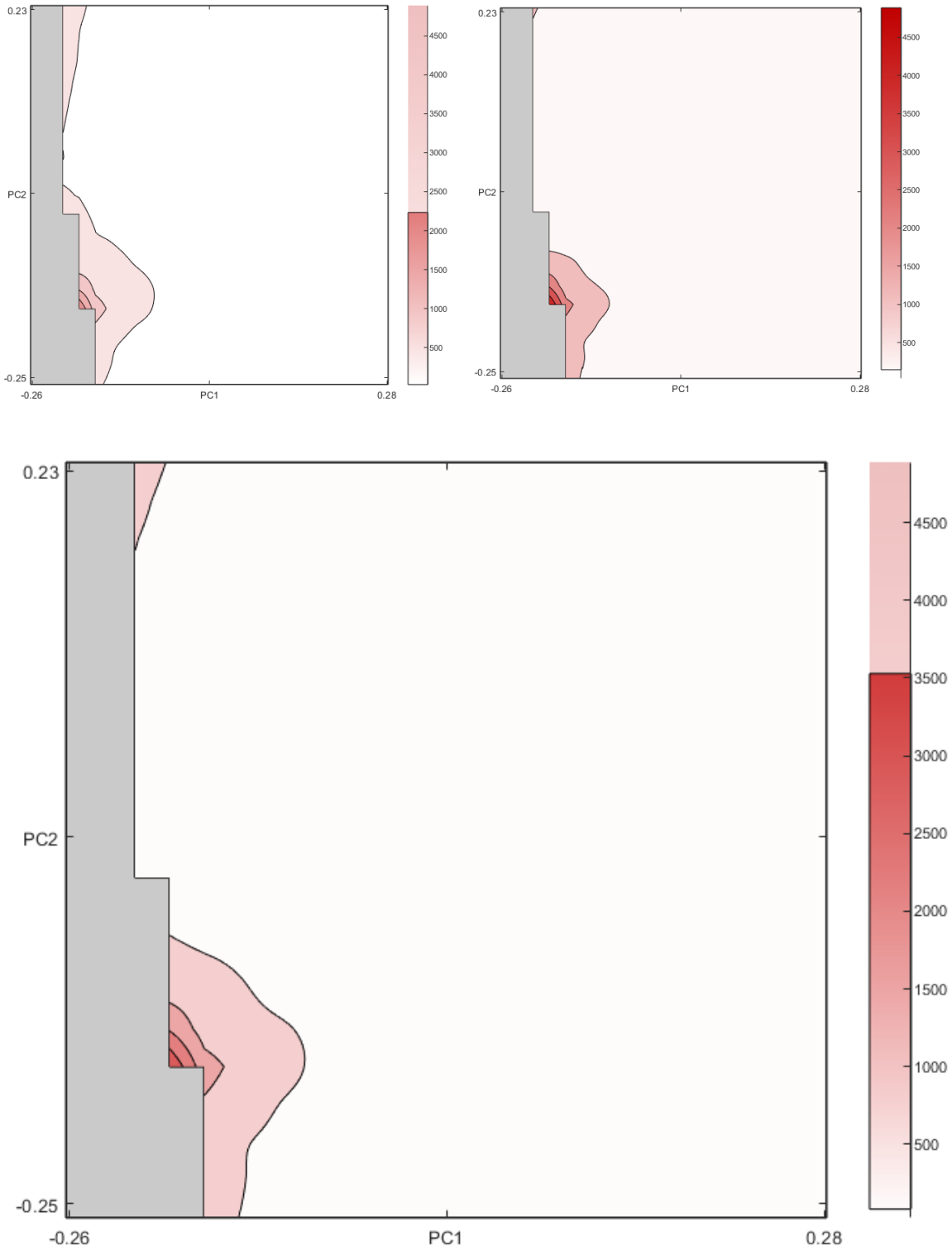


Fig S7: Von Mises Stress (VMS) surface plots. Top left: 5th percentile result of 1000 randomised inputs. Top right: 95th percentile result of 1000 randomised inputs. Bottom: mean result of 1000 randomised inputs.

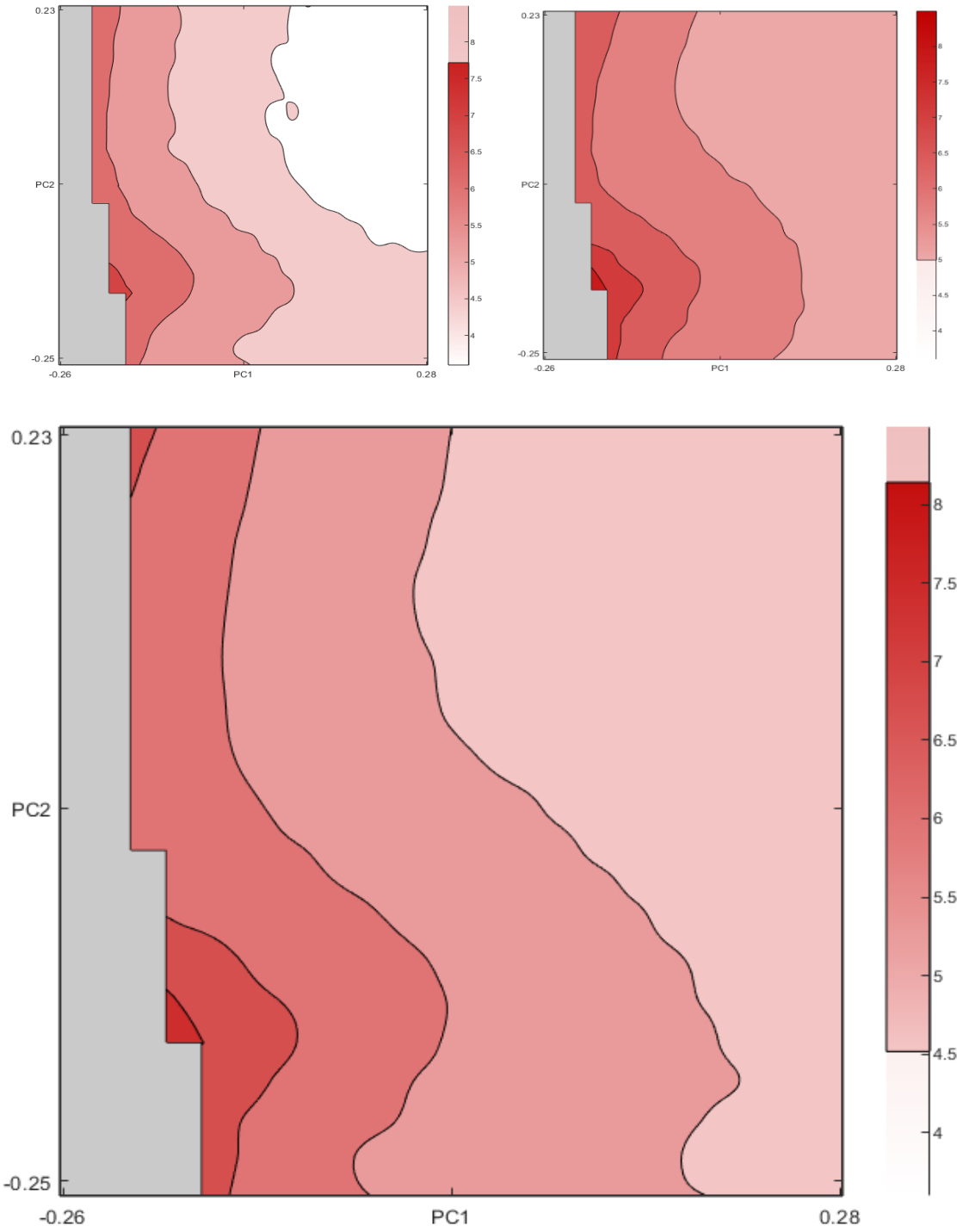


Fig S8: Log scaled Von Mises Stress (log VMS) surface plots. Top left: 5th percentile result of 1000 randomised inputs. Top right: 95th percentile result of 1000 randomised inputs. Bottom: mean result of 1000 randomised inputs.

Phylogeny

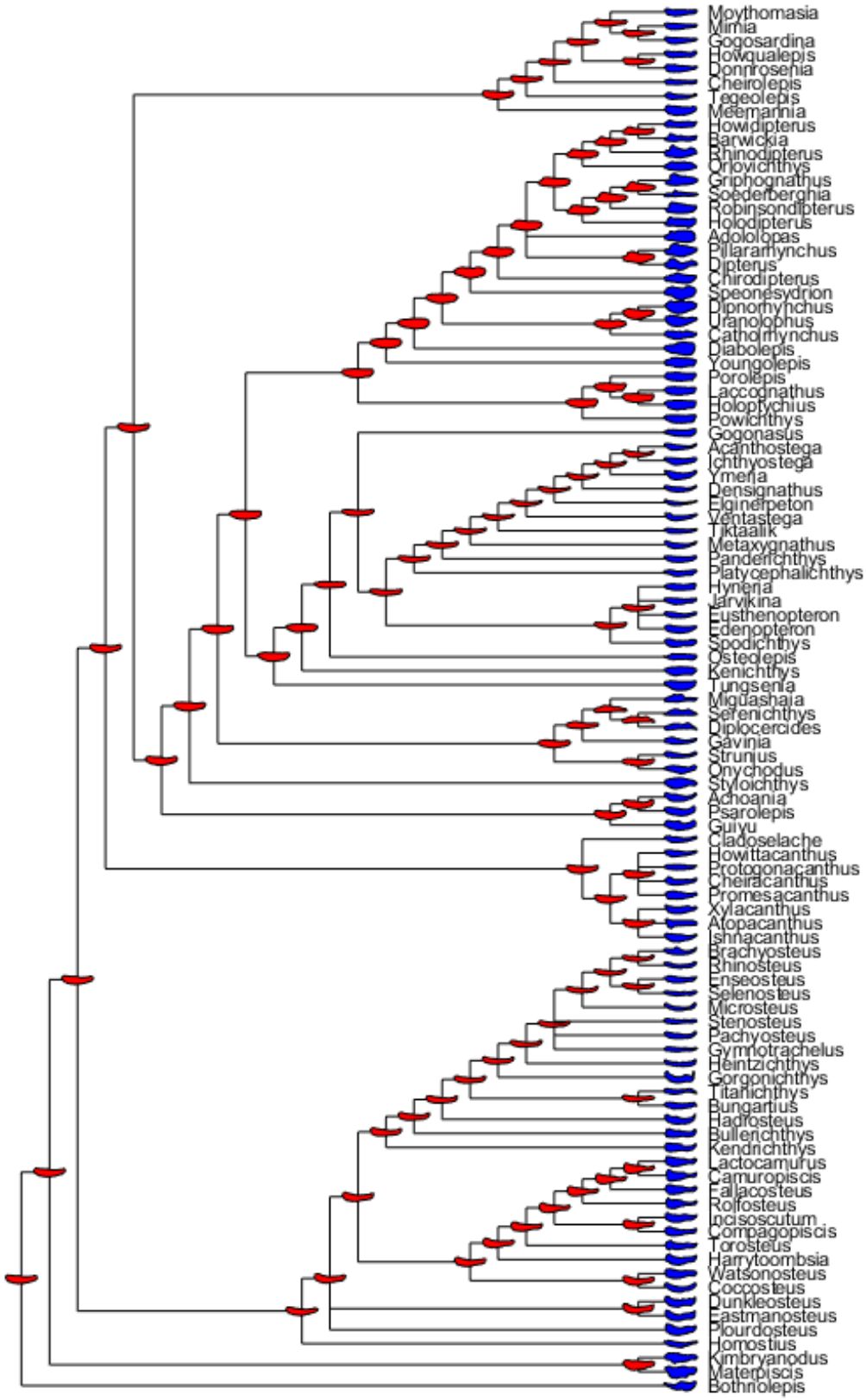


Fig S9: Phylogeny with taxon jaw shapes and ancestral jaw shapes superimposed. Blue shapes = empirical jaw shapes of sample taxa, red shapes = reconstructed jaw shapes output from ancestral state reconstruction.

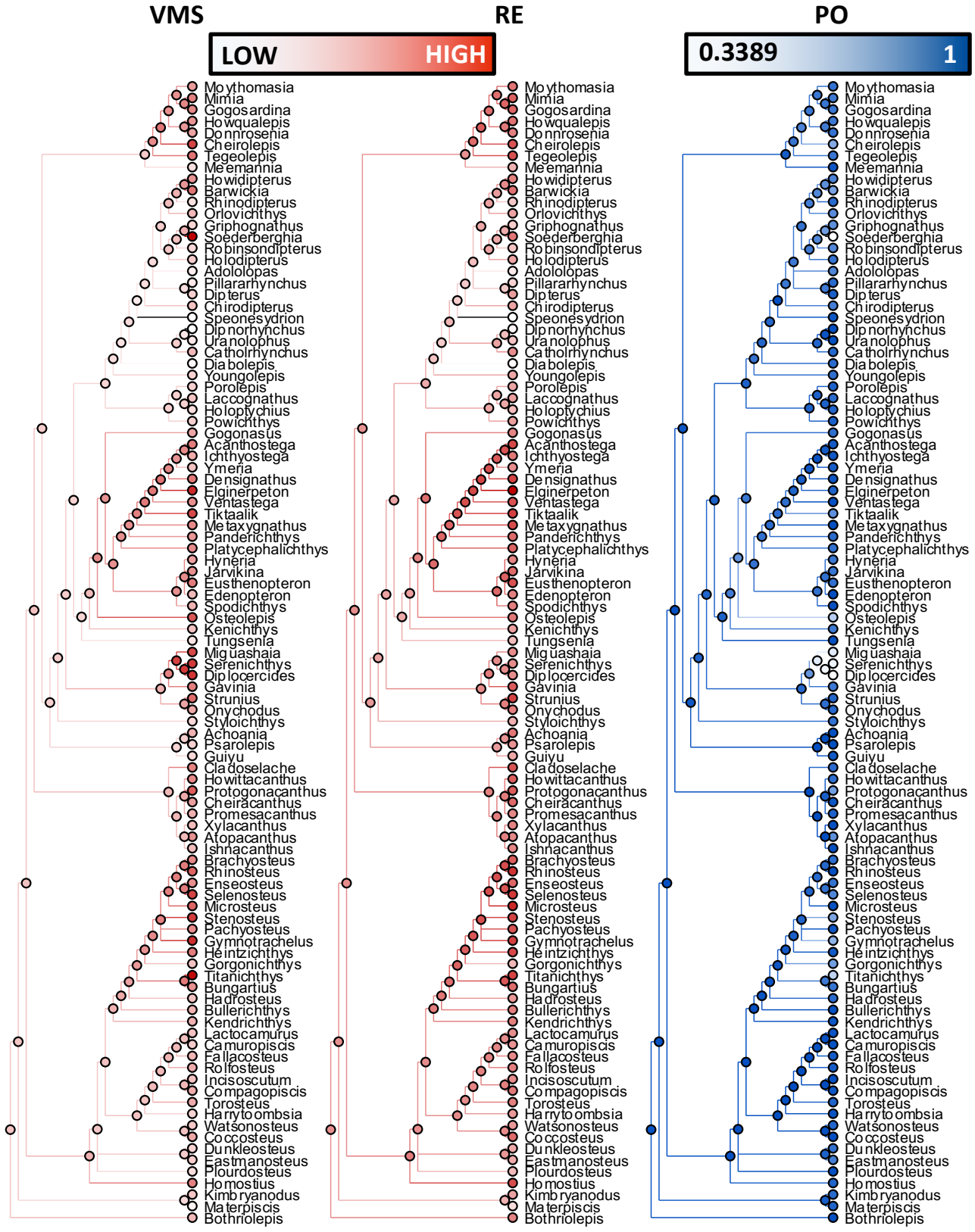
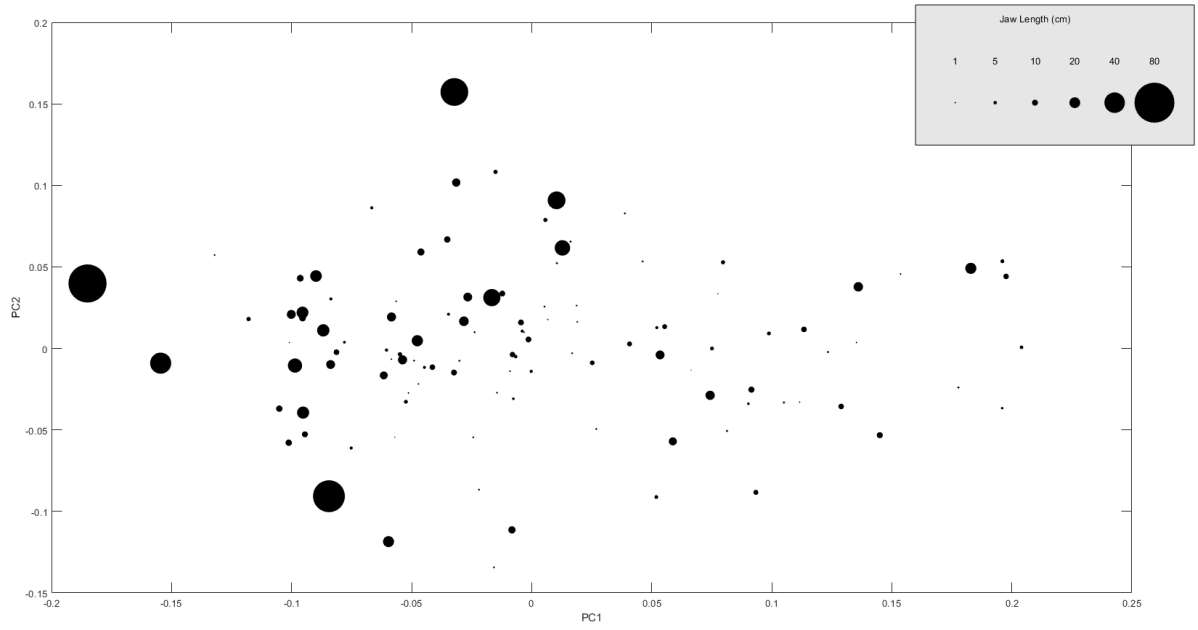
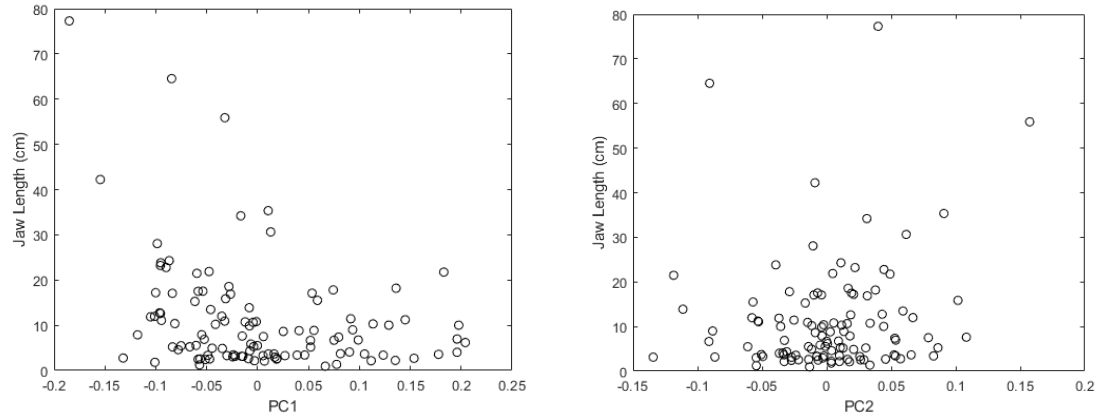


Fig S10: Phylogeny with extrapolated performance values (shades of red) and optimality values (shades of blue) superimposed. Coloured circles represent values of individual nodes (both empirical taxa and inferred ancestral states). VMS = Von Mises Stress; RE = Rotational Efficiency; PO = Pareto Optimality.





Fig

S11: Relationship between jaw length and shape. Longer Jaws appear to be biased towards lower PC1 values, but all PC2 values. Shorter jaws are less restricted in shape than longer jaws. A PGLS shows a significant relationship between jaw length and PC1 ($p = 0.04129$, R-squared = 0.03485), and no significant relationship between length and PC2 ($p = 0.4846$, R-squared = 0.0056).

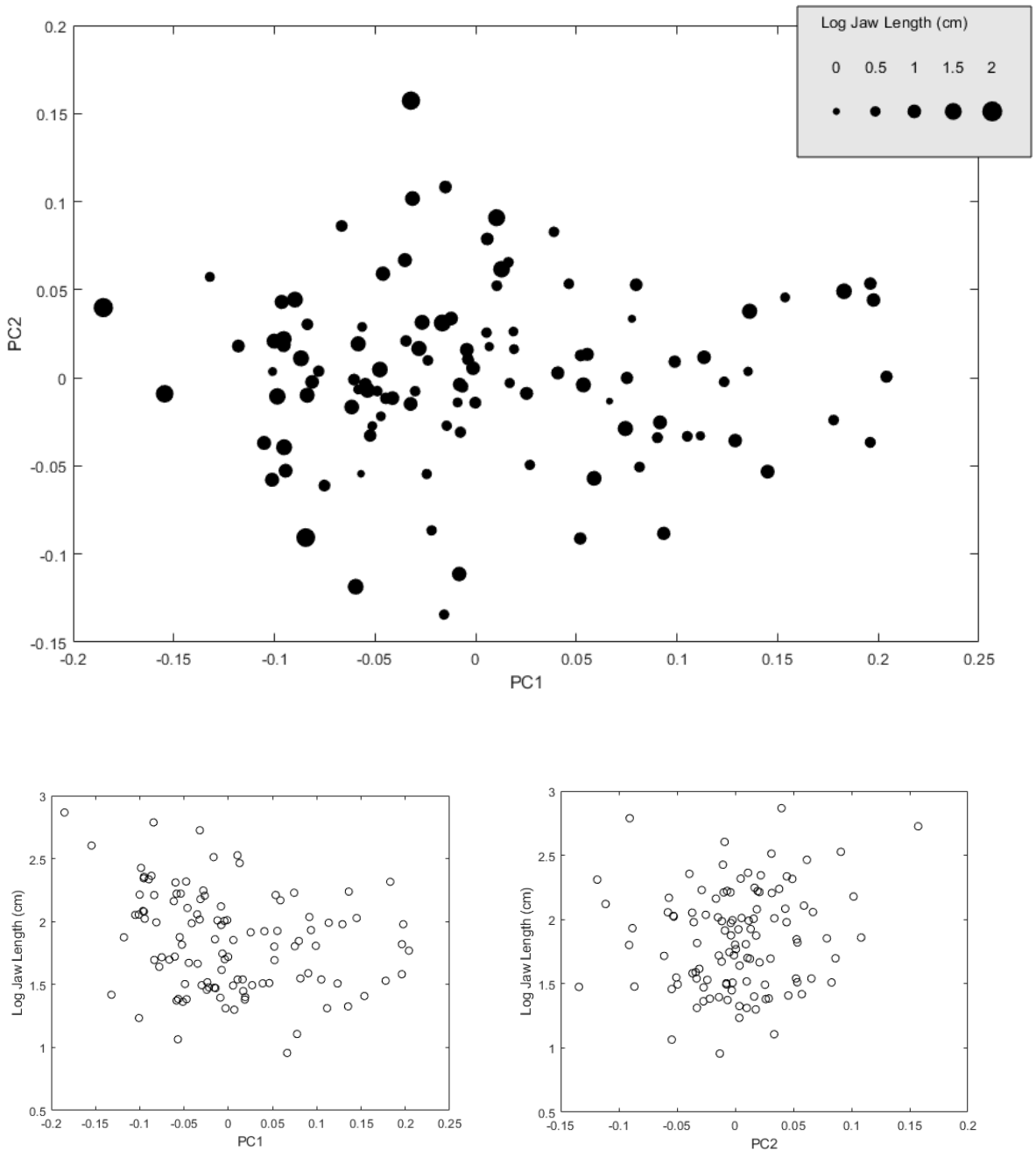


Fig S12: Relationship between log jaw length and shape. A PGLS shows a significant relationship between jaw length and PC1 ($p = 0.00462$, R-squared = 0.0627), and no significant relationship between length and PC2 ($p = 0.3191$, R-squared = 0.00954).

Data S1: Data sources, polynomial fit of performance surfaces, and disparity metrics

Data S1A: Sources of mandible morphology data

Index Number	Genus	First Appearance	Last Appearance	Clade	Image Type	Image Source
1	*Acanthostega*	Frasnian	Famennian	Sarcopterygii	Reconstruction	(*83*)
2	*Achoania*	Lochkovian	Lochkovian	Sarcopterygii	Specimen Photograph	(*84*)
3	*Adololopas*	Frasnian	Frasnian	Sarcopterygii	Specimen Photograph	(*85*)
4	*Angarichthys*	Eifelian	Givetian	Placodermi	Specimen Photograph	(*86*)
5	*Arquatichthys*	Pragian	Pragian	Sarcopterygii	Specimen Drawing	(*87*)
6	*Atopacanthus*	Givetian	Givetian	Chondrichthyes	Specimen Photograph	(*88*)
7	*Barwickia*	Givetian	Frasnian	Sarcopterygii	Reconstruction	(*89*)
8	*Bothriolepis*	Frasnian	Famennian	Placodermi	µCT Scan	(*90*)
9	*Brachydeirus*	Frasnian	Frasnian	Placodermi	Specimen Photograph	NHM: 53180
10	*Brachyosteus*	Frasnian	Frasnian	Placodermi	Reconstruction	(*91*)
11	*Brontichthys*	Famennian	Famennian	Placodermi	Specimen Photograph	CMNH: 7575
12	*Bullerichthys*	Frasnian	Frasnian	Placodermi	Specimen Photograph	WAM: 869703
13	*Bungartius*	Famennian	Famennian	Placodermi	Specimen Drawing	(*92*)
14	*Camuropiscis*	Frasnian	Frasnian	Placodermi	Specimen Photograph	(*5*)
15	*Cathlorhynchus*	Lochkovian	Eifelian	Sarcopterygii	Specimen Photograph	(*93*)
16	*Cavanosteus*	Emsian	Emsian	Placodermi	Specimen Photograph	ANU: V77
17	*Cheiracanthus*	Eifelian	Givetian	Chondrichthyes	Specimen Photograph	UCMZ: 1132
18	*Cheirolepis*	Emsian	Frasnian	Actinopterygii	Specimen Photograph	MNB: 5112
19	*Chirodipterus*	Frasnian	Frasnian	Sarcopterygii	Specimen Photograph	MNB: 12875a
20	*Cladoselache*	Famennian	Famennian	Chondrichthyes	Specimen Drawing	(*94*)
21	*Coccosteus*	Eifelian	Givetian	Placodermi	Specimen Photograph	(*95*)
22	*Compagopiscis*	Frasnian	Frasnian	Placodermi	µCT Scan	(*90*)
23	*Copanognathus*	Frasnian	Frasnian	Placodermi	Specimen Drawing	(*96*)
24	*Denisonodus*	Frasnian	Frasnian	Placodermi	Specimen Photograph	(*97*)
25	*Densignathus*	Famennian	Famennian	Sarcopterygii	Reconstruction	(*98*)
26	*Diabolepis*	Lochkovian	Lochkovian	Sarcopterygii	Specimen Photograph	(*99*)
27	*Diplocercides*	Givetian	Frasnian	Sarcopterygii	Reconstruction	(*100*)
28	*Diplognathus*	Famennian	Famennian	Placodermi	Reconstruction	(*91*)
29	*Dipnorhynchus*	Emsian	Emsian	Sarcopterygii	Specimen Photograph	NHM: 46773

30	*Dipterus*	Famennian	Famennian	Sarcopterygii	Specimen Photograph	NHM: P34552
31	*Donnrosenia*	Givetian	Givetian	Actinopterygii	Specimen Photograph	(*72*)
32	*Dunkleosteus*	Famennian	Famennian	Placodermi	Specimen Photograph	(*5*)
33	*Eastmanosteus*	Givetian	Famennian	Placodermi	Specimen Photograph	(*5*)
34	*Edenopteron*	Famennian	Famennian	Sarcopterygii	Reconstruction	(*101*)
35	*Elginerpeton*	Frasnian	Frasnian	Sarcopterygii	Reconstruction	(*83*)
36	*Enseosteus*	Frasnian	Frasnian	Placodermi	Specimen Photograph	MNB: 18318
37	*Erromenosteus*	Frasnian	Frasnian	Placodermi	Specimen Photograph	MNB: 139
38	*Eusthenopteron*	Givetian	Famennian	Sarcopterygii	Reconstruction	(*102*)
39	*Fallacosteus*	Frasnian	Frasnian	Placodermi	Specimen Photograph	(*5*)
40	*Gavinia*	Eifelian	Givetian	Sarcopterygii	Reconstruction	(*103*)
41	*Gogonasus*	Frasnian	Frasnian	Sarcopterygii	Specimen Photograph	(*104*)
42	*Gogosardina*	Frasnian	Frasnian	Actinopterygii	Specimen Photograph	(*105*)
43	*Gorgonichthys*	Famennian	Famennian	Placodermi	Specimen Photograph	(*5*)
44	*Griphognathus*	Frasnian	Frasnian	Sarcopterygii	Specimen Photograph	ANU: 21186
45	*Guiyu*	Silurian	Silurian	Sarcopterygii	Specimen Photograph	(*70*)
46	*Gymnotrachelus*	Famennian	Famennian	Placodermi	Specimen Photograph	CMNH: 8051
47	*Hadrosteus*	Frasnian	Frasnian	Placodermi	Reconstruction	(*91*)
48	*Harrytoombsia*	Frasnian	Frasnian	Placodermi	Specimen Photograph	WAM: 704254
49	*Heintzichthys*	Frasnian	Famennian	Placodermi	Specimen Photograph	(*106*)
50	*Holodipterus*	Frasnian	Frasnian	Sarcopterygii	Reconstruction	(*100*)
51	*Holodus*	Frasnian	Frasnian	Sarcopterygii	Specimen Drawing	(*107*)
52	*Holoptychius*	Givetian	Famennian	Sarcopterygii	Specimen Photograph	(*108*)
53	*Homostius*	Emsian	Givetian	Placodermi	Specimen Photograph	(*109*)
54	*Howidipterus*	Frasnian	Frasnian	Sarcopterygii	Reconstruction	(*89*)
55	*Howittacanthus*	Givetian	Givetian	Chondrichthyes	Specimen Drawing	(*110*)
56	*Howqualepis*	Givetian	Givetian	Actinopterygii	Specimen Drawing	(*111*)
57	*Hussakofia*	Famennian	Famennian	Placodermi	Specimen Photograph	CMNH: 8082
58	*Hyneria*	Famennian	Famennian	Sarcopterygii	Specimen Drawing	(*112*)
59	*Ichthyostega*	Famennian	Famennian	Sarcopterygii	Reconstruction	(*83*)
60	*Incisoscutum*	Frasnian	Frasnian	Placodermi	Specimen Photograph	(*106*)

61	*Ishnacanthus*	Silurian	Eifelian	Chondrichthyes	Specimen Photograph	(*113*)
62	*Jarvikina*	Givetian	Famennian	Sarcopterygii	Specimen Photograph	(*114*)
63	*Kendrichthys*	Frasnian	Frasnian	Placodermi	Specimen Photograph	NHM: P51143
64	*Kenichthys*	Emsian	Emsian	Sarcopterygii	Reconstruction	(*84*)
65	*Kimbryanodus*	Frasnian	Frasnian	Placodermi	Specimen Photograph	(*115*)
66	*Laccognathus*	Givetian	Frasnian	Sarcopterygii	Specimen Photograph	(*116*)
67	*Lactocamurus*	Frasnian	Frasnian	Placodermi	Specimen Photograph	(*5*)
68	*Latvius*	Givetian	Frasnian	Sarcopterygii	Reconstruction	MNB: f551
69	*Leptosteus*	Frasnian	Frasnian	Placodermi	Specimen Photograph	MNB: 12709
70	*Malerosteus*	Frasnian	Frasnian	Placodermi	Specimen Photograph	(*117*)
71	*Materpiscis*	Frasnian	Frasnian	Placodermi	Specimen Drawing	(*118*)
72	*Meemannia*	Lochkovian	Lochkovian	Actinopterygii	Specimen Drawing	(*119*)
73	*Megamastax*	Silurian	Silurian	Sarcopterygii	Specimen Photograph	(*120*)
74	*Metaxygnathus*	Famennian	Famennian	Sarcopterygii	Reconstruction	(*83*)
75	*Microsteus*	Frasnian	Frasnian	Placodermi	Specimen Photograph	MNB: 18324
76	*Miguashaia*	Givetian	Frasnian	Sarcopterygii	Reconstruction	(*121*)
77	*Mimia*	Frasnian	Frasnian	Actinopterygii	Reconstruction	(*84*)
78	*Moythomasia*	Givetian	Famennian	Actinopterygii	Specimen Drawing	NHM: P53221
79	*Mylostoma*	Famennian	Famennian	Placodermi	Specimen Photograph	CMNH: 7706
80	*Nesides*	Frasnian	Frasnian	Sarcopterygii	Reconstruction	(*103*)
81	*Onychodus*	Emsian	Famennian	Sarcopterygii	Reconstruction	(*103*)
82	*Orlovichthys*	Famennian	Famennian	Sarcopterygii	Specimen Drawing	(*122*)
83	*Osteolepis*	Eifelian	Givetian	Sarcopterygii	Specimen Photograph	UCMZ: GN769
84	*Oxyosteus*	Frasnian	Frasnian	Placodermi	Specimen Photograph	MNB: 296
85	*Pachyosteus*	Frasnian	Famennian	Placodermi	Specimen Photograph	MNB: 389
86	*Paledaphus*	Frasnian	Famennian	Sarcopterygii	Specimen Photograph	AMNH: 6560
87	*Panderichthys*	Givetian	Frasnian	Sarcopterygii	Specimen Drawing	(*83*)
88	*Pholidosteus*	Frasnian	Frasnian	Placodermi	Specimen Photograph	MNB: 12797
89	*Pillararhynchus*	Frasnian	Frasnian	Sarcopterygii	Specimen Photograph	(*123*)
90	*Platycephalichthys*	Frasnian	Frasnian	Sarcopterygii	Reconstruction	(*7*)
91	*Plourdosteus*	Givetian	Frasnian	Placodermi	Specimen Photograph	(*124*)

92	*Porolepis*	Lochkovian	Pragian	Sarcopterygii	Specimen Photograph	(*125*)
93	*Powichthys*	Lochkovian	Lochkovian	Sarcopterygii	Reconstruction	(*126*)
94	*Promesacanthus*	Lochkovian	Lochkovian	Chondrichthyes	Specimen Drawing	(*127*)
95	*Protogonacanthus*	Frasnian	Famennian	Chondrichthyes	Reconstruction	(*128*)
96	*Psarolepis*	Silurian	Lochkovian	Sarcopterygii	Specimen Photograph	(*84*)
97	*Ptyctodus*	Eifelian	Famennian	Placodermi	Specimen Photograph	(*96*)
98	*Rhinodipterus*	Frasnian	Famennian	Sarcopterygii	Specimen Photograph	(*123*)
99	*Rhinosteus*	Frasnian	Frasnian	Placodermi	Reconstruction	(*91*)
100	*Robinsondipterus*	Frasnian	Frasnian	Sarcopterygii	Specimen Photograph	WAM: 011003
101	*Rolfosteus*	Frasnian	Frasnian	Placodermi	Specimen Photograph	NHM: P50971
102	*Selenosteus*	Frasnian	Famennian	Placodermi	Specimen Photograph	CMNH: 8086
103	*Serenichthys*	Famennian	Famennian	Sarcopterygii	Reconstruction	(*129*)
104	*Soederberghia*	Frasnian	Famennian	Sarcopterygii	Reconstruction	(*100*)
105	*Speonesydrion*	Pragian	Pragian	Sarcopterygii	Specimen Photograph	ANU: 35647
106	*Spodichthys*	Frasnian	Frasnian	Sarcopterygii	µCT Scan	(*130*)
107	*Stenognathus*	Frasnian	Frasnian	Placodermi	Specimen Drawing	(*96*)
108	*Stenosteus*	Frasnian	Famennian	Placodermi	Specimen Photograph	CMNH: 8044
109	*Strunius*	Givetian	Famennian	Sarcopterygii	Specimen Photograph	MNB: 161b
110	*Styloichthys*	Lochkovian	Lochkovian	Sarcopterygii	Specimen Photograph	(*84*)
111	*Tegeolepis*	Frasnian	Famennian	Actinopterygii	Specimen Photograph	NHM: P45312
112	*Tiktaalik*	Frasnian	Frasnian	Sarcopterygii	Specimen Photograph	(*131*)
113	*Titanichthys*	Famennian	Famennian	Placodermi	Specimen Photograph	(*132*)
114	*Torosteus*	Frasnian	Frasnian	Placodermi	Specimen Photograph	WAM: 8863
115	*Tungsenia*	Pragian	Pragian	Sarcopterygii	Reconstruction	(*133*)
116	*Uranolophus*	Pragian	Eifelian	Sarcopterygii	Specimen Photograph	FMNH: PF3874
117	*Ventastega*	Famennian	Famennian	Sarcopterygii	Specimen Drawing	(*83*)
118	*Watsonosteus*	Eifelian	Givetian	Placodermi	Specimen Drawing	(*134*)
119	*Xylacanthus*	Silurian	Pragian	Chondrichthyes	Specimen Photograph	(*135*)
120	*Ymeria*	Frasnian	Famennian	Sarcopterygii	Reconstruction	(*136*)
121	*Youngolepis*	Lochkovian	Pragian	Sarcopterygii	Reconstruction	(*84*)

Abbreviation	Institution
NHM	Natural History Museum, London, UK

MNB	Museum für Naturkunde, Berlin, Germany
CMNH	Cleveland Museum of Natural History, Cleveland, OH, USA
WAM	Western Australian Museum, Perth, Australia
ANU	Australian National University, Canberra, Australia
UCMZ	University of Cambridge Museum of Zoology, Cambridge, UK
FMNH	The Field Museum, Chicago, IL, USA
AMNH	American Museum of natural History, New York, NY, USA

Data S1B: Second order polynomial fit to Rotational Efficiency (RE) and Von Mises Stress (VMS) surface

Equation:

	RE	RE 5% ci	RE 95% ci	VMS	VMS 5% ci	VMS 95% ci
p_C	1.805	1.8	1.81	255.5	225.6	285.5
p_x	-0.7324	-0.755	-0.7099	-1783	-1914	-1652
p_y	-0.04755	-0.06746	-0.02764	-734.9	-850.6	-619.3
p_{xx}	1.308	0.8923	1.185	5205	4356	6054
p_{xy}	-0.1133	-0.2447	0.01808	3364	2600	4127
p_{yy}	-1.837	-1.977	-1.697	1046	234	1858

Goodness of Fit:

	RE	VMS
SSE	0.3619	12210000
R^2	0.928	0.6669
Adjusted R^2	0.9272	0.663
RMSE	0.02929	170.1191

Data S1C: Spearman rank correlation test for trend over time (* = significant at p < 0.05)

	Sum of Variances	Mean Pairwise Distance	Mean Optimality
rho	0.6667	0.8810*	-0.9286*
p	0.0831	0.0072	0.0022

Data S1D: Pearson's linear rank test of disparity metrics against mean optimality (* = significant at p < 0.05)

	Sum of Variances	Mean Pairwise Distance
r	-0.5476	-0.7619*

p	0.171	0.0368

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