

Supplementary Table 1. Eigenvectors representing the weights of the individual geometric invariants towards the first four principal components.

Geometric Invariants ^a	Principal Components			
	PC1	PC2	PC3	PC4
Edges				
d _{1,4}	-0.191	0.286	0.183	-0.095
d _{2,5}	-0.219	0.202	-0.009	0.004
d _{3,6}	-0.222	-0.015	-0.174	0.098
d _{4,7}	-0.213	-0.220	-0.024	-0.003
d _{5,8}	-0.187	-0.282	0.219	-0.107
d _{1,7}	-0.209	0.086	-0.269	-0.229
d _{2,8}	-0.208	-0.082	-0.271	-0.232
d _{1,8}	-0.209	0.007	-0.244	-0.303
Perimeter				
Triangle _{1,5,8} (P _{1,5,8})	-0.239	0.025	-0.067	-0.234
Tetrahedron _{1,2,3,4} (P _{1,2,3,4})	-0.193	0.311	0.181	-0.035
Tetrahedron _{2,3,4,5} (P _{2,3,4,5})	-0.221	0.219	-0.023	0.104
Tetrahedron _{3,4,5,6} (P _{3,4,5,6})	-0.226	-0.023	-0.177	0.194
Tetrahedron _{4,5,6,7} (P _{4,5,6,7})	-0.217	-0.249	-0.011	0.071
Tetrahedron _{5,6,7,8} (P _{5,6,7,8})	-0.188	-0.307	0.221	-0.060
Tetrahedron _{1,3,5,7} (P _{1,3,5,7})	-0.243	0.080	-0.136	-0.120
Tetrahedron _{2,4,6,8} (P _{2,4,6,8})	-0.241	-0.086	-0.144	-0.119
Area				
Triangle _{1,5,8} (A _{1,5,8})	-0.154	0.025	0.361	-0.006
Volume				
Tetrahedron _{1,2,3,4} (V _{1,2,3,4})	0.134	-0.185	-0.243	0.098
Tetrahedron _{2,3,4,5} (V _{2,3,4,5})	0.154	-0.181	-0.156	0.032
Tetrahedron _{3,4,5,6} (V _{3,4,5,6})	0.160	-0.062	0.049	-0.113
Tetrahedron _{4,5,6,7} (V _{4,5,6,7})	0.159	0.109	0.041	-0.052
Tetrahedron _{5,6,7,8} (V _{5,6,7,8})	0.149	0.216	-0.183	0.096
Tetrahedron _{1,3,5,7} (V _{1,3,5,7})	-0.057	-0.018	0.272	-0.068
Tetrahedron _{2,4,6,8} (V _{2,4,6,8})	-0.061	0.007	0.343	-0.128
Sum of product of centroid to node distances.				
Tetrahedron _{1,2,3,4} (SP _{1,2,3,4})	-0.138	0.296	0.146	0.178
Tetrahedron _{2,3,4,5} (SP _{2,3,4,5})	-0.162	0.211	-0.020	0.401
Tetrahedron _{3,4,5,6} (SP _{3,4,5,6})	-0.167	-0.030	-0.131	0.499
Tetrahedron _{4,5,6,7} (SP _{4,5,6,7})	-0.159	-0.255	0.024	0.341
Tetrahedron _{5,6,7,8} (SP _{5,6,7,8})	-0.134	-0.303	0.205	0.125

^aSee the legend to figure 1 for description of the individual geometric invariants.