**Supplementary Material from D.C. Adams and M.L. Collyer, “Multivariate phylogenetic comparative methods: evaluations, comparisons, and recommendations”. *Systematic Biology*.**

**1: Multivariate LRT and AIC tests: Additional Evaluations**

Here we present results from additional computer simulations evaluating model misspecification when using AIC comparisons based on the full multivariate log-likelihood (sensu Revell and Harmon 2008). For these simulations, multivariate datasets were generated under a Brownian motion model of evolution, with no input covariation between trait dimensions. Next, the fit of the data to the phylogeny was obtained under both Brownian motion and an Orstein-Uhlenbeck models, and AIC scores for each were obtained. These were then compared to determine which model provided the highest support. Simulations were performed at differing levels of species richness (*N* = 32, 64, 128) as well as for differing numbers of trait dimensions (*p* = 4, 8, 12). Evolutionary model comparisons were performed in both the *mvMORPH* and *mvSLOUCH* packages.

*Results.* Both implementations of the procedure displayed high levels of model misspecification. Using *mvMORPH*, model misspecification increased as trait dimensionality increased, attaining levels of nearly 50% for *N* = 32 and *p* = 12 (Fig. SM1a). When the number of taxa increased there was no noticeable decrease in model misspecification, but levels remained high at around 15% (Fig. SM1b). Using *mvSLOUCH* there were much higher levels of model misspecification under initial conditions (~50%), but levels paradoxically decreased as trait dimensionality increased (Fig. SM1c). However, and also paradoxically, model misspecification increased sharply as the number of taxa was increased, attaining levels of nearly 90% (Fig. SM1d). Overall these results demonstrate that for both implementations, model misspecification rates are unacceptably high when comparing differing evolutionary models.

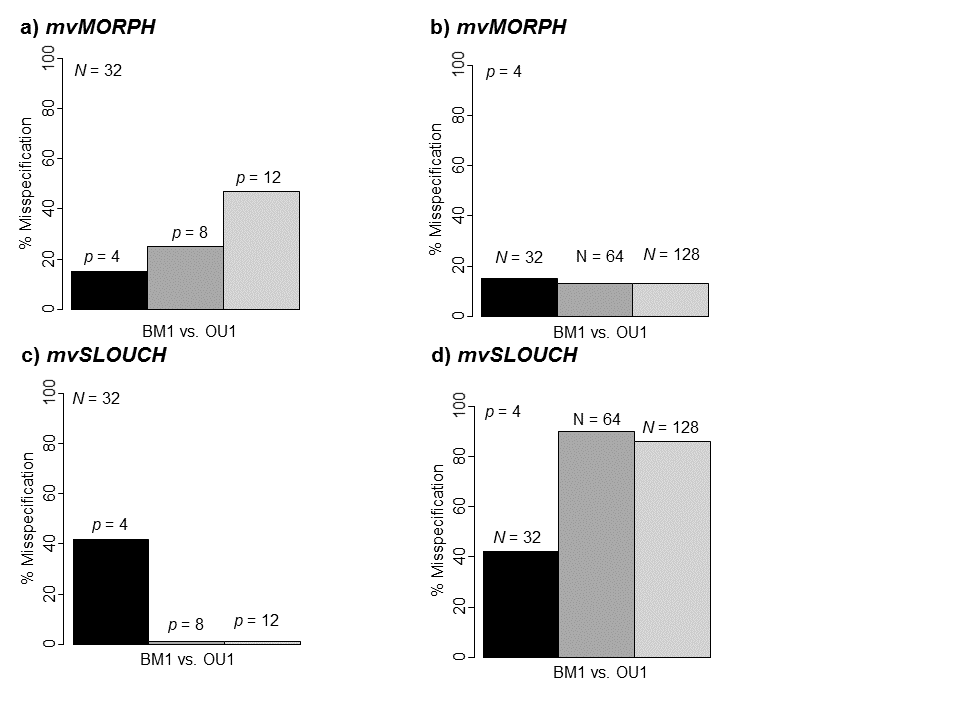


Fig. SM1. Results from statistical simulations evaluating the percent model misspecification based on comparisons of evolutionary models. For all scenarios, data were simulated under a Brownian motion model of evolution, and both BM and OU models were compared. Percent model misspecification using the *mvMORPH* package as a) trait dimensionality increases, and b) as the number of taxa in the phylogeny increases. Percent model misspecification using the *mvSLOUCH* package as c) trait dimensionality increases, and d) as the number of taxa in the phylogeny increases.

**2: Additional Simulation Results: Trait Covariation and Rotation Effects**

Here we present results from additional computer simulations demonstrating the geometric properties of different multivariate phylogenetic comparative methods. As described in the text, simulations were performed on 100 phylogenies containing 32 species each. Phylogenies were generated using both random-splits and pure-birth procedures. Next, on each phylogeny a 16-dimensional phenotype was simulated under Brownian motion. Four sets of simulations were performed, each using a different level of input covariation among trait dimensions (0.0, 0.3, 0.6, 0.9). We then performed two different rotations on each simulated dataset to provide views of each in different orientations. The first rotation was performed by aligning the data to its principal component axes, while the second was accomplished by generating a random rotation matrix and rotating the dataset to an arbitrary orientation. Finally, an additional simulation was performed in which the number of trait dimensions was systematically increased (*p* = 6, 8, 10, 12, 14, 16, 18, 20, 22, 24, 26, 28, 30, 32).

Using these datasets we performed several comparisons of multivariate comparative approaches. First we obtained the multivariate log-likelihood (log*L*) describing the fit of the data to its respective phylogeny under Brownian motion for all datasets in all three orientations: original, PCA-rotated, and arbitrarily-rotated. Likewise, we estimated the pairwise composite likelihood (PCL) score all datasets in all three orientations. We then performed a series of Pearson product-moment correlations between log*L* and PCL values to determine the extent to which PCL was a faithful representation of the true multivariate log*L* at differing levels of trait covariation, and to determine the effect of dataspace orientation on estimates of log*L* and PCL.

*Results: logL vs. logL.* For both random-splits and pure-birth phylogenies, the correlation between log*L* values across orientations was precisely 1.0, regardless of levels of trait covariation or how the data were rotated (Table SM1). These results confirm that the multivariate log*L* is insensitive to data orientation and levels of covariation across trait dimensions.

Table SM1. Results of simulations comparing multivariate log*L* across differing orientations. Values represent the Pearson product-moment correlation found from log*L* scores across 100 simulated datasets represented in different orientations.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | Random-Splits Phylogenies | | | |  | Pure-Birth Phylogenies | | | |
| Ycov | 0.0 | 0.3 | 0.6 | 0.9 |  | 0.0 | 0.3 | 0.6 | 0.9 |
| Orig vs. PCA | 1.0 | 1.0 | 1.0 | 1.0 |  | 1.0 | 1.0 | 1.0 | 1.0 |
| Orig vs. Arbitrary | 1.0 | 1.0 | 1.0 | 1.0 |  | 1.0 | 1.0 | 1.0 | 1.0 |

*Results: logL vs. PCL.* For both random-splits and pure-birth phylogenies, the correlation between log*L* and PCL values across different orientations was less than one in all cases. Further, as levels of trait covariation increased, the correlation between the two decreased (Table SM2). These findings reveal that there was not a one-to-one correspondence between PCL and the multivariate log*L*, implying that PCL is not a faithful representation of the actual multivariate log*L.*

Table SM2. Results of simulations comparing multivariate log*L* to PCL. Values represent the Pearson product-moment correlation found from log*L* and PCL scores across 100 simulated datasets.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | Random-Splits Phylogenies | | | |  | Pure-Birth Phylogenies | | | |
| Ycov | 0.0 | 0.3 | 0.6 | 0.9 |  | 0.0 | 0.3 | 0.6 | 0.9 |
| R | 0.908 | 0.757 | 0.608 | 0.482 |  | 0.991 | 0.948 | 0.934 | 0.871 |

*Results: PCL vs. PCL.* For both random-splits and pure-birth phylogenies, the correlation between PCL values across different orientations was less than one in all cases. Further, as levels of trait covariation increased, the correlation between PCL estimates decreased (Table SM3). Because the general trends were the same for both principal components and arbitrary rotations, these results reveal that PCL is sensitive to the orientation of the dataset regardless of the method used to rotate the dataspace. Additionally, these effects were worse as levels of trait covariation increased.

Table SM3. Results of simulations comparing PCL estimates across differing orientations. Values represent the Pearson product-moment correlation found from PCL values across 100 simulated datasets represented in different orientations.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | Random-Splits Phylogenies | | | |  | Pure-Birth Phylogenies | | | |
| Ycov | 0.0 | 0.3 | 0.6 | 0.9 |  | 0.0 | 0.3 | 0.6 | 0.9 |
| Orig vs. PCA | 0.923 | 0.817 | 0.542 | 0.462 |  | 0.989 | 0.955 | 0.919 | 0.871 |
| Orig vs. Arbitrary | 0.996 | 0.913 | 0.816 | 0.767 |  | 0.999 | 0.989 | 0.977 | 0.905 |

*Results: PCL vs. PCL with increasing trait dimension.* For both random-splits and pure-birth phylogenies, the correlation between PCL values across different orientations was less than one in all cases. Further, the correlation between PCL estimates for datasets with large numbers of trait dimensions were generally lower than those with smaller numbers of trait dimensions, when comparing datasets in their original and PCA orientation (Table SM4). With arbitrary rotations patterns were more varied, but in all cases the correlation was considerably less than 1.0. Thus, the overall patterns revealed that PCL was negatively affected by trait dimensionality in addition to trait covariation and dataset orientation.

Table SM4. Results of simulations comparing PCL estimates across differing orientations for different numbers of trait dimensions (*p*). Values represent the Pearson product-moment correlation found from PCL values across 100 simulated datasets represented in different orientations. PC designates comparisons between the original data and those rotated to their principal component axes. AC designates comparisons between the original data and those rotated arbitrarily.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | Random-Splits Phylogenies | | | | | | | | | | | | |  |
| *p* | 6 | 8 | 10 | 12 | 14 | 16 | 18 | 20 | 22 | 24 | 26 | 28 | 30 | 32 |
| PC | 0.702 | 0.671 | 0.646 | 0.590 | 0.502 | 0.497 | 0.508 | 0.627 | 0.538 | 0.498 | 0.400 | 0.391 | 0.496 | 0.290 |
| AR | 0.787 | 0.801 | 0.807 | 0.792 | 0.794 | 0.848 | 0.779 | 0.861 | 0.810 | 0.818 | 0.832 | 0.861 | 0.813 | 0.869 |
|  | Pure-Birth Phylogenies | | | | | | | | | | | | |  |
| *p* | 6 | 8 | 10 | 12 | 14 | 16 | 18 | 20 | 22 | 24 | 26 | 28 | 30 | 32 |
| PC | 0.933 | 0.961 | 0.924 | 0.936 | 0.935 | 0.923 | 0.888 | 0.882 | 0.910 | 0.896 | 0.882 | 0.863 | 0.864 | 0.832 |
| AR | 0.787 | 0.801 | 0.807 | 0.792 | 0.794 | 0.848 | 0.779 | 0.861 | 0.810 | 0.818 | 0.832 | 0.861 | 0.813 | 0.869 |

**3: Singularity of multivariate log*L* for GM shape data**

Here we present results illustrating that the multivariate log*L* cannot be computed for data that themselves display redundancies, such as is observed using landmark-based geometric morphometric data. Here, a set of landmark coordinates serve as the original source of morphological characterization, and these are subsequently subjected to a Procrustes analysis to remove the effects of non-shape variation (specimen position, orientation, and scale), resulting in a set of aligned Procrustes coordinates. This multidimensional dataset perfectly describes the shape of objects as measured by the original landmarks, but contains redundancies as a result of Procrustes superimposition. The computer code below performs such an analysis, and subsequently demonstrates that such data cannot be used in its original form for the purposes of obtaining the multivariate log*L* fit of the data to the phylogeny under a particular evolutionary model. The example is shown in its entirety, and the computer code is found in the additional materials on DRYAD.

> library(geomorph)

>

> #Revell & Harmon 2008 logL for multivariate data

> StandardLogL<-function(phy,x){

+ x<-as.matrix(x)

+ N<-nrow(x)

+ p<-ncol(x)

+ C<-vcv.phylo(phy)

+ C<-C[rownames(x),rownames(x)]

+ a<-colSums(solve(C))%\*%x/sum(solve(C))

+ D<-matrix(0,N\*p,p)

+ for(i in 1:(N\*p)) for(j in 1:p) if((j-1)\*N<i&&i<=j\*N) D[i,j]=1.0

+ y<-as.matrix(as.vector(x))

+ one<-matrix(1,N,1)

+ R<-t(x-one%\*%a)%\*%solve(C)%\*%(x-one%\*%a)/N

+ L1<- -(t(y-D%\*%t(a))%\*%solve(kronecker(R,C))%\*%(y-D%\*%t(a))/2)-N\*p\*log(2\*pi)/2-determinant(kronecker

+ (R,C))$modulus[1]/2

+ return(list(LogL=L1,sigma=R))

+ }

> data("plethspecies")

> Y.gpa<-gpagen(plethspecies$land[1:3,,]) #use only 3 landmarks

|====================================================================| 100%

> x<-two.d.array(Y.gpa$coords)

> phy<-plethspecies$phy

> StandardLogL(phy,x)

Error in solve.default(kronecker(R, C)) :

system is computationally singular: reciprocal condition number = 3.17418e-20

Called from: solve.default(kronecker(R, C))

> #Why this fails: R is singular

> x<-as.matrix(x)

> N<-nrow(x); p<-ncol(x)

> C<-vcv.phylo(phy); C<-C[rownames(x),rownames(x)]

> a<-colSums(solve(C))%\*%x/sum(solve(C))

> D<-matrix(0,N\*p,p)

> for(i in 1:(N\*p)) for(j in 1:p) if((j-1)\*N<i&&i<=j\*N) D[i,j]=1.0

> y<-as.matrix(as.vector(x))

> one<-matrix(1,N,1)

> R<-t(x-one%\*%a)%\*%solve(C)%\*%(x-one%\*%a)/N

> solve(R)

Error in solve.default(R) :

system is computationally singular: reciprocal condition number = 9.57883e-20

**4: Comparison of R-code implementations of algebraic generalizations of PCMs as found in *geomorph* (written by the original authors of those approaches), and in *phylocurve.* Here we present results for computation time comparisons under various scenarios. The algorithms used in *phylocurve* were suggested to be substantially improved, in terms of computation time; however, this is only true in rare circumstances. We summarize results below and provide raw results, subsequently.**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Function comparison | Comparable Constraints | When is phylocruve faster?\* | When are the two comparable?\* | When is geomorph faster?\* | Comments |
| procD.pgls | * phylocruve does not allow RRPP * phylocurve only works with phylogenetic regression * phylocurve has limited output available for downstream analyses | 500 or more species, with fewer traits than species | Fewer than 500 species and fewer traits than species | All HD cases | * The phylocurve version of this function will work with multiple independent variables, but will return incorrect results. The function was not designed for complex models but does not trap multiple variables. |
| Noticeable coding Errors   * Recursive strategy used in permutation procedure * Elimination of observed values from sampling distributions, making first random cases the observed values. * (See annotated script for specific details.) |
| compare.evol.rates |  | In no cases | Most species and most traits, especially when traits were fewer than species | Greater than 250 species and greater than 50 traits | * The phylocurve version has an option for choosing between ML or REML methods. This determined whether rates were averaged by *N* or *N*-1 degrees of freedom, respectively. |
| compare.multi.evol.rates |  | Small advantage at 500 species | 100 or fewer traits / 250 or fewer species | Small disadvantage for HD scenarios with 250 -500 traits | * The phylocurve version has an option for choosing between ML or REML methods. This determined whether rates were averaged by *N* or *N*-1 degrees of freedom, respectively. |
| physignal | * geomorph only offers *Kmult*; phylocurve offers *Kmult* and *SSC*. | Small advantage at 500 species | 250 or fewer traits / 250 or fewer species | Small disadvantage HD data such as 500 traits for 50-250 species |  |
| phylo.integration | * phylocurve is limted to non HD data | In no cases | Most cases except large species/large trait cases | Large species/large trait cases | * phylocurve functions tended to throw errors due to non-convergence in fortran. Simulations were censored because of such errors. |

\* All computation summaries are based on a 6 × 6 table of outcomes comparing computation time between analogous functions of geomorph and phylocurve. The column and row headers for this table comprise the number of species and traits used, respectively, including 10, 24, 50, 100, 250, 500. Computation times were the mean of three separate runs on the same simulated data. Analyses were run with 500 and 1,000 random permutations, which were considered sufficient for elucidating meaningful differences in computation time, and found to be rather consistent in results. Any computation time comparison that resulted in a one-second or less difference was considered comparable (see below). Meaningful differences are bolded and color-coded to highlight the instances where the methods diverge. All details are available in the R-script, geomorph.phylocurve.time.trials.R.

procD.pgls (500 permutations): geomorph - phylocurve, seconds

10.species 24.species 50.species 100.species 250.species 500.species

10.traits -0.02332717 -0.01706449 -0.010498421 0.04345693 0.4371393 **2.262797**

24.traits -0.03102146 -0.01959969 -0.006179409 0.11799019 0.8757337 **4.407458**

50.traits -0.03992620 -0.04442155 -0.004264628 0.17488603 **1.5876317 7.890903**

100.traits -0.08082275 -0.11280637 0.010325354 0.21104186 **2.9044345 13.657260**

250.traits -0.51150765 -0.71908304 -0.907085417 -0.42822153 **2.8119507 25.344876**

500.traits **-2.00463317 -2.95343682 -4.218838473 -6.18257397** 0.9418458 **19.242847**

procD.pgls (1000 permutations): geomorph - phylocurve, seconds

10.species 24.species 50.species 100.species 250.species 500.species

10.traits -0.05049307 -0.09122400 -0.001685146 0.08557626 0.8800662 **3.761320**

24.traits -0.05504121 -0.09791768 -0.001341708 0.19542437 **1.7233049 7.823575**

50.traits -0.07529529 -0.08926141 0.015691439 0.35681031 **3.2794761 15.691074**

100.traits -0.22309545 -0.15454156 0.025430358 0.24508598 **5.7344932 26.822344**

250.traits **-1.22361704 -1.65117674 -1.736390783** -0.89933245 **5.8027640 45.541804**

500.traits **-5.24835601 -6.48768081 -8.598580567 -11.18316410** 0.7967663 **34.403779**

compare.evol.rates (500 permutations): geomorph - phylocurve, seconds

10.species 24.species 50.species 100.species 250.species 500.species

10.traits -0.11083295 -0.12888565 -0.1786679 -0.3062459 **-1.201949 -4.588913**

24.traits -0.10270200 -0.13470699 -0.1495203 -0.3550863 **-2.152833 -4.836343**

50.traits -0.09913663 -0.13121825 -0.2078117 -0.6282985 **-2.255284 -6.834146**

100.traits -0.11006732 -0.52900391 -0.3601948 -0.7619709 **-3.416232 -12.172651**

250.traits -0.12990616 -0.09383219 -0.3869218 **-1.5435002 -7.014134 -26.600044**

500.traits 0.65522541 0.43912477 -0.4425127 **-1.2657184 -13.237516 -48.741774**

compare.evol.rates (1000 permutations): geomorph - phylocurve, seconds

10.species 24.species 50.species 100.species 250.species 500.species

10.traits -0.1968703 -0.2529047 -0.2873316 -0.6661536 **-3.060519 -9.423560**

24.traits -0.2033470 -0.3302040 -0.3834433 -0.9556864 **-4.190398 -21.265493**

50.traits -0.2201437 -0.3384667 -0.4796197 -0.7821626 **-5.591487 -7.434048**

100.traits -0.2482425 -0.3308941 -0.5852791 **-1.6453698 -6.797260 -17.324970**

250.traits -0.1391346 -0.6180336 **-1.5150193 -5.8613471 -13.044101 -114.470787**

500.traits **1.0418778** -0.3375493 0.8161278 **-16.9499650 -9.155061 -93.938453**

compare.multi.evol.rates (500 permutations): geomorph - phylocurve, seconds

10.species 24.species 50.species 100.species 250.species 500.species

10.traits -0.05049990 -0.08611792 -0.07152327 0.006134703 0.3259109 **2.333843**

24.traits -0.07786592 -0.08914974 -0.04943136 0.031761963 0.4289184 **3.059883**

50.traits -0.11650066 -0.10171709 -0.13296940 -0.052302866 **1.6455324 4.629210**

100.traits -0.47726823 -0.09487975 -0.17397429 0.074969961 **1.4278640 6.215576**

250.traits **-4.79639628 -4.99100767 -4.36066428** -0.771729368 **1.8574633 11.641120**

500.traits **-28.36199561 -33.47482239 -21.61948158 -11.723661045 -4.6274501** **22.701828**

compare.multi.evol.rates (1000 permutations): geomorph - phylocurve, seconds

10.species 24.species 50.species 100.species 250.species 500.species

10.traits -0.09716823 -0.1325108 -0.1137868 -0.07027595 0.7883642 3.094634

24.traits -0.10784990 -0.1681266 -0.3383144 -0.15892938 **1.9048460 6.083778**

50.traits -0.16886379 0.1056515 -0.1612323 0.11074079 0.5419862 **17.331242**

100.traits -0.54491605 -0.5259155 -0.2022365 0.09130198 **4.9874745 12.078983**

250.traits **-4.82567798 -6.4460668 -0.7117952 -1.67120742** **3.5191351 50.308199**

500.traits **-33.74271705 -43.9419840 -33.3373977 -3.43052295**  -0.4673147 **402.192025**

physignal (500 pemrutations): geomorph - phylocurve, seconds

10.species 24.species 50.species 100.species 250.species 500.species

10.traits -0.01097556 -0.009927137 0.003513197 0.05146831 0.5319463 **3.125528**

24.traits -0.01138539 -0.013806917 0.020016404 0.10879542 **1.0710226 5.125866**

50.traits -0.03442819 -0.038306457 -0.032500844 0.14458930 **1.8330007 9.431531**

100.traits -0.09233469 -0.166630159 -0.149782456 0.05759362 **2.9573192 15.858265**

250.traits -0.59145082 -0.969112396 **-1.342344621 -1.59561683** **2.1352392 24.621676**

500.traits **-2.59955652 -4.348743321 -5.799665191 -8.99152451 -11.4999881** **18.884567**

physignal (1000 permutations): geomorph - phylocurve, seconds

10.species 24.species 50.species 100.species 250.species 500.species

10.traits -0.02211436 -0.01392492 -0.005453799 0.11456972 **1.042440 4.574499**

24.traits -0.02594808 -0.01284100 0.037557131 0.33580616 **1.910059 8.291457**

50.traits -0.05724429 -0.07464378 0.028356115 0.21288981 **3.205015 15.177472**

100.traits -0.18199385 -0.22888147 -0.237686117 0.01904137 **5.054781 27.226137**

250.traits -0.90852210 **-1.48730030 -2.335488238 -3.92289979** **3.676002 47.028627**

500.traits **-4.27940335 -6.39004061 -12.431019550 -17.80472655 -20.441645** **34.807091**

phylo.integration 500 permutations: geomorph - phylocurve, seconds

10.species 24.species 50.species 100.species 250.species 500.species

10.traits -0.02190446 -0.02839539 -0.03649802 -0.0606490 -0.03100767 0.48641792

24.traits -0.08820138 -0.06163742 -0.09129689 -0.1461887 -0.34996251 -0.09460487

50.traits -0.33364703 -0.36821290 -0.24703083 -0.4720621 **-1.17805841 -1.83437239**

phylo.integration (1000 permutations): geomorph - phylocurve, seconds

10.species 24.species 50.species 100.species 250.species 500.species

10.traits -0.03157956 -0.09714189 -0.06978678 -0.1034685 -0.1401521 0.7104906

24.traits -0.16573852 -0.14527012 -0.25343760 -0.3299903 -0.7282639 **-1.0774785**

50.traits -0.81751854 -0.93022575 -0.37870494 -0.9849263 **-2.1985922 -4.4740088**