Appendix

A1 More complex models of trait evolution

In the main text we examined the performance of the four indices of phylogenetic signal and their associated tests only under Brownian motion trait evolution. It remained open, how different models of trait evolution would modify the results and the recommendations drawn from them. Here, we provide some additional results for a selection of more complex models of trait evolution. We did not include these in the sensitivity analysis, because we did not have quantitative hypotheses for phylogenetic signal given the different models and thus could not compare results to expectations. Furthermore, suggested models of trait evolution and their possible parameterizations are too numerous for a comprehensive comparison. However, it is worth exploring whether and in which directions the main results are affected for some commonly used models of trait evolution.

To this end, we performed additional simulations with different models of evolution (scenarios with branch lengths, no polytomies and 100 species): we accounted for Ornstein-Uhlenbeck models (function ouTree in geiger), 'speciational' models (kappaTree) and models that slow-down or speed-up the rate of character evolution over evolutionary time (deltaTree). The Ornstein-Uhlenbeck model describes a random walk with a central tendency (in our case the trait value of the respective ancestor) of strength α (with $\alpha = 0$ describing pure Brownian motion). Increasing values describe increasing influence of the ancestral value. The theoretical expectation for trait value distribution among the phylogeny for increasing α is a decreasing phylogenetic signal (Revell, Harmon & Collar 2008). Note, that this relates to the controversy about how to measure phylogenetic niche conservatism, i.e. the tendency of related species to retain their ancestral niches (Wiens & Graham 2005). It has been proposed that phylogenetic niche conservatism can be identified by high phylogenetic signal (Losos

2008) even so simulation studies have shown that strong niche conservatism may lead to patterns of very low phylogenetic signal (Revell, Harmon & Collar 2008).

The slow-down or speed-up models correspond to evolutionary rates that decrease or increase in dependence on evolutionary time with strength δ (see Tab. A1b). The parameter δ equal to one describes pure Brownian motion, smaller values to slow-down and larger values to speed-up. The theoretical expectation for trait value distribution among the phylogeny for increasing δ is a decreasing phylogenetic signal (Pagel 1999). The speciation model corresponds to evolutionary rates that depend on original branch lengths with strength κ and simulates punctual versus gradual evolution (see Tab. A1b). The parameter κ equal to one describes pure Brownian motion and decreasing values describe increasingly stronger speciation. The theoretical expectation for trait value distribution among the phylogeny for increasing κ is an increasing phylogenetic signal (Pagel 1999).

Table A1: Phylogenetic signal indices and tests (a) and related measures (b)

(a) Phylogenetic signal indices and tests

Index	**Short description**	**R-function (package)**	**References**
PICs	A special case of a phylogenetic generalized least squares model. Differences in trait values of sister nodes are standardized by square root of sum of respective branch length. Resulting contrasts are statistically independent.	pic3 (picante) pic (ape)	(Felsenstein, 2008; Felsenstein, 1985)
Cheverud's comparative method	A variance decomposition approach. The total variance of a trait across species is separated into an ancestral and a specific part using a maximum likelihood procedure.	compar.cheverud (ape)	(Cheverud, Dow & Leutenegger 1985)
Lynch's comparative method	Fits the heritable (additive) component, the residual (specific) component and their variance/covariance structure in a mixed model for trait distribution using an expectation maximization algorithm. Phylogenetic heritability is mathematically equivalent to Pagel's λ.	compar.lynch (ape)	(Lynch 1991)
Moran's *I*	Measures the autocorrelation of trait values based on phylogenetic distance.	moran.I (ape) gearymoran (ade4) moran.idx (adephylo) abouheif.moran	(Gittleman & Kot, 1990)
Abouheif's C_{mean}	Measures the autocorrelation of trait values of neighbor taxa.	abouheif.moran with method Abouheif (adephylo)	(Abouheif, 1999)
Blomberg's *K*	Sets the mean squared error of the tip data (measured from the phylogenetic corrected mean) in relation to the mean squared error based on the variance-covariance matrix derived from the phylogeny. The stronger the effect of phylogenetic relatedness, the higher the ratio.	phylogsignal (geiger) phylosig (phytools)	(Blomberg, Garland & Ives 2003; Revell 2012)
Geary's *c*	Measures the autocorrelation of trait values based on phylogenetic distance. Inversely correlated to Moran's I, but more sensitive to autocorrelation at small scales.	abouheif.moran with method Abouheif (adephylo)	(Geary 1954; Revell 2012)
Pagel's *λ*	Parameter that scales the expected covariances of trait values (as inferred from the phylogenetic relationships) down to the actually observed ones. It thus reflects the ancestral part of variance in the trait distribution. Fitted via a maximum likelihood approach.	fitContinuous (geiger) gls with correlation structure corPagel (nlme, ape) phylosig (phytools) pgls(caper)	(Pagel 1999; Revell 2012)

(b) Indices related to phylogenetic signal

Index	Short description	R-function (package)	References
felsen	A unit of squared evolutionary changes. It describes the change of one unit in the variance among sister taxa of ln-transformed trait values.	pic3 (picante) fitContinuous (geiger)	(Ackerly 2009)
SkR2k	Performs the orthonormal decomposition of variance of a quantitative variable to compare variance explained by internal nodes with variance explained by end nodes. The higher the internal node variance, the higher the phylogenetic signal.	orthogram (adephylo)	(Ollier, Couteron & Chessel 2006)
R2Max	The maximum value of squared correlations between a quantitative trait and the resulting vectors of a variance decomposition procedure into phylogenetic and specific components. High values indicate a strong influence of local trait changes (at one node) for the overall trait distribution.		
Dmax	Tests for a smooth distribution of the resulting vectors of the variance decomposition, i.e. whether variance adds up uniformly in a sequence of nodes.		
SCE	Similar to *Dmax*. Tests for the local variation of the orthogram and for the average local variation of orthogram values, i.e. the change between neighbors.		
Pagel's κ	A measures for punctual versus gradual evolution. Branch lengths are raised to the power of κ: if evolution is punctual, the information content of branch length is low and κ approaches zero (i.e. all branches are scaled to unity). κ is fitted using a maximum likelihood approach.	fitContinuous (geiger) pgls(caper)	(Pagel 1999)
Pagel's δ	A measure for the rate of evolution has accelerated or slowed down over time. Node depths are raised to the power of δ: if evolution is faster in older branches, δ takes values smaller 1 and vice versa. δ is fitted using a maximum likelihood approach.		
Pavoine's S_1	Based on the decomposition of trait diversity (measured by the quadratic entropy index) among the nodes of a phylogenetic. The single-node skewness test identifies, whether a single node in the tree drives trait diversity.	R-functions are available in the supplementary material of the reference paper	(Pavoine, Baguette & Bonsall 2010)
Pavoine's S_2	The few-node skewness test determines, whether only a few nodes have an exceptional high contribution to trait diversity.		
Pavoine's S_3	The tips/roots skewness test identifies whether phylogenetic skewness is biased towards the tips or the root. The authors suggest that this test is related to the phylogenetic signal test of Blomberg et al. (2003).		

Tables A2

Tables show the influence of explanatory variables (rows) on response variables (columns). The first column for each response variable shows estimates for effect sizes of the explanatory variables, the second column shows significance levels (*p*, *<0.05, **<0.01, ***<0.001) estimated with a GAM. Please note that these *p*-values should only be used to compare the strength of effects between different simulation scenarios with an equal number of repetitions (*p*-values may become significant even for very small effect sizes due to high sample size in simulation experiments and are thus not useful to identify important effects per se). Response variables are averaged over repetition and include phylogenetic signal indices (A2a), standard deviations of phylogenetic signal indices (A2b), ranks of observed values in the null model distributions (A2c) and standard deviations of ranks of observed values in the null model distributions (A2d) each for Abouheif 's C_{mean}, Moran's I, Blomberg's K and Pagel's λ. Effect sizes were calculated as the coefficients of variation of the average response in the groups defined by the explanatory variables. Significance was calculated by model comparison of the full model and a model missing the focal explanatory variable. The full model used splines for smoothing the effect of the strength of Brownian motion (w) and the number of species (N) as main and interaction effects. The explanatory variables polytomies (P) and branch length information (B) only have two values (yes and no). Transformations of the response variable and degrees of freedom for the splines were chosen based on visual residual analyses (for details see footnotes of the tables).

Table A2a: Phylogenetic signal indices

	Abouheif's C_{mean}		**Moran's *I***		**Blomberg's *K***		**Pagel's λ**	
	effect size	*p*	*effect size*	*p*	*effect size*	*p*	*effect size*	*p*
w	0.83	***	1.03	***	0.85	***	0.75	***
N	0.16	***	0.21	***	0.19	***	0.03	***
P	0.01	-	0.00	-	0.03	-	0.01	-
BL	0.00	-	0.07	***	0.68	***	0.07	***
w : N	0.81	***	1.02	***	0.84	**	0.72	***
w : P	0.81	-	1.00	-	0.83	-	0.73	-
w : BL	0.81	-	1.01	***	1.00	***	0.73	***
N : P	0.15	-	0.19	-	0.18	-	0.03	-
N : BL	0.15	-	0.24	***	0.54	***	0.06	-
P : BL	0.01	-	0.06	**	0.56	***	0.06	-

Transformations: square root transformation for Blomberg's *K*, arcus-sinus square root transformation for Pagel's λ; Degrees of freedom for smoothing: 5 df for main effects and 3 df for interactions

Table A2b: Standard deviations of phylogenetic signal indices

	Abouheif's C_{mean}		**Moran's *I***		**Blomberg's *K***		**Pagel's λ**	
	effect size	*p*	*effect size*	*p*	*effect size*	*p*	*effect size*	*p*
w	0.42	***	0.54	***	1.13	***	0.51	***
N	0.11	***	0.47	***	0.16	***	0.06	***
P	0.01	-	0.00	-	0.08	-	0.00	-
BL	0.00	-	0.32	**	0.60	***	0.02	***
w : N	1.09	-	1.09	***	1.24	***	1.32	-
w : P	0.41	-	0.53	***	1.11	-	0.50	-
w : BL	0.41	-	0.57	***	1.53	-	0.58	***
N : P	0.10	-	0.44	-	0.17	-	0.06	-
N : BL	0.10	**	0.50	***	0.49	***	0.06	***
P : BL	0.00	-	0.26	-	0.50	***	0.02	-

Transformations: log transformation for Abouheif 's C_{mean}, Moran's I and Blomberg's *K*, arcus-sinus square root transformation for Pagel's λ; Degrees of freedom for smoothing: 3df for main effects and interactions

Table A2c: Phylogenetic signal tests

	Abouheif's C_{mean}		**Moran's *I***		**Blomberg's *K***		**Pagel's λ**	
	effect size	p	effect size	p	effect size	p	effect size	p
w	1.31	***	1.31	***	1.10	***	1.21	***
N	0.34	**	0.37	***	0.17	***	0.41	**
P	0.03	-	0.01	-	0.06	-	0.01	-
BL	0.01	-	0.06	-	0.17	***	0.05	-
w : N	1.35	***	1.35	***	1.08	***	1.28	***
w : P	1.28	-	1.27	-	1.08	***	1.18	-
w : BL	1.28	-	1.28	**	1.09	***	1.18	-
N : P	0.32	-	0.35	-	0.16	-	0.39	-
N : BL	0.32	-	0.35	-	0.21	***	0.39	-
P : BL	0.02	-	0.05	-	0.15	**	0.05	-

Transformations: sqrt transformation for Abouheif 's C_{mean}, Moran's *I*, Blomberg's *K*and Pagel's λ; Degrees of freedom for smoothing: 3df for main effects and interactions

Table A2d: Standard deviations of phylogenetic signal tests

	Abouheif's C_{mean}		**Moran's *I***		**Blomberg's *K***		**Pagel's λ**	
	effect size	p	effect size	p	effect size	p	effect size	p
w	1.10	***	1.10	***	0.96	***	0.91	***
N	0.21	***	0.22	***	0.08	***	0.21	**
P	0.03	-	0.01	-	0.03	-	0.00	-
BL	0.01	-	0.04	-	0.14	***	0.05	-
w : N	1.27	***	1.26	***	0.96	-***	1.16	***
w : P	1.07	-	1.07	-	0.94	***	0.89	-
w : BL	1.07	-	1.08	***	0.97	***	0.89	-
N : P	0.20	-	0.21	-	0.08	-	0.20	-
N : BL	0.20	-	0.22	*	0.15	***	0.20	-
P : BL	0.03	-	0.03	-	0.12	**	0.04	-

Transformations: sqrt transformation for Abouheif 's C_{mean}, Moran's *I*, Blomberg's *K*and Pagel's λ; Degrees of freedom for smoothing: 3df for main effects and interactions

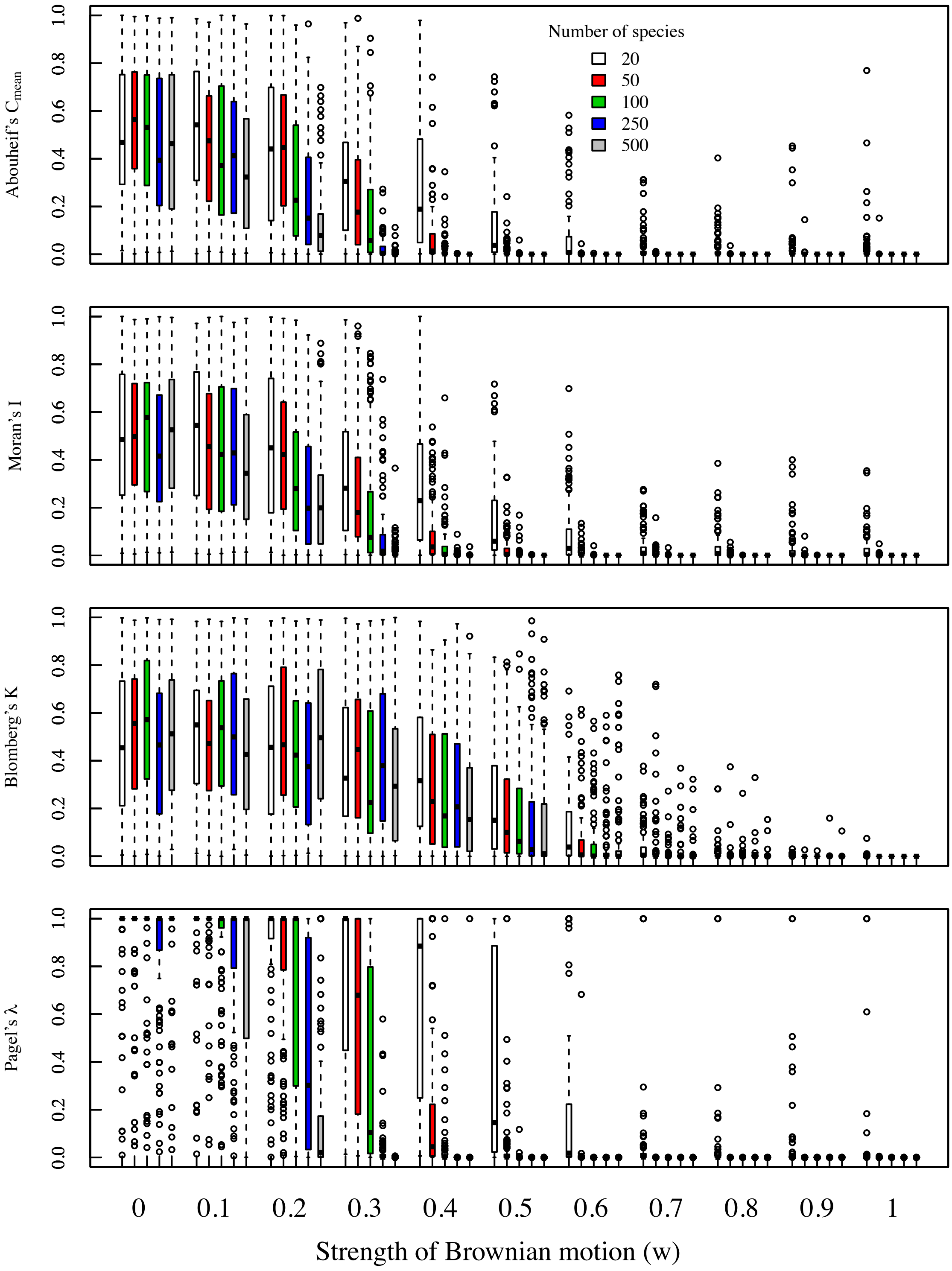

Figure A1

Response of phylogenetic signal tests (*p*-values for observed values given the null model distributions) to increasing strength of Brownian motion for different sample sizes (shown are scenarios with branch length information and no polytomies).

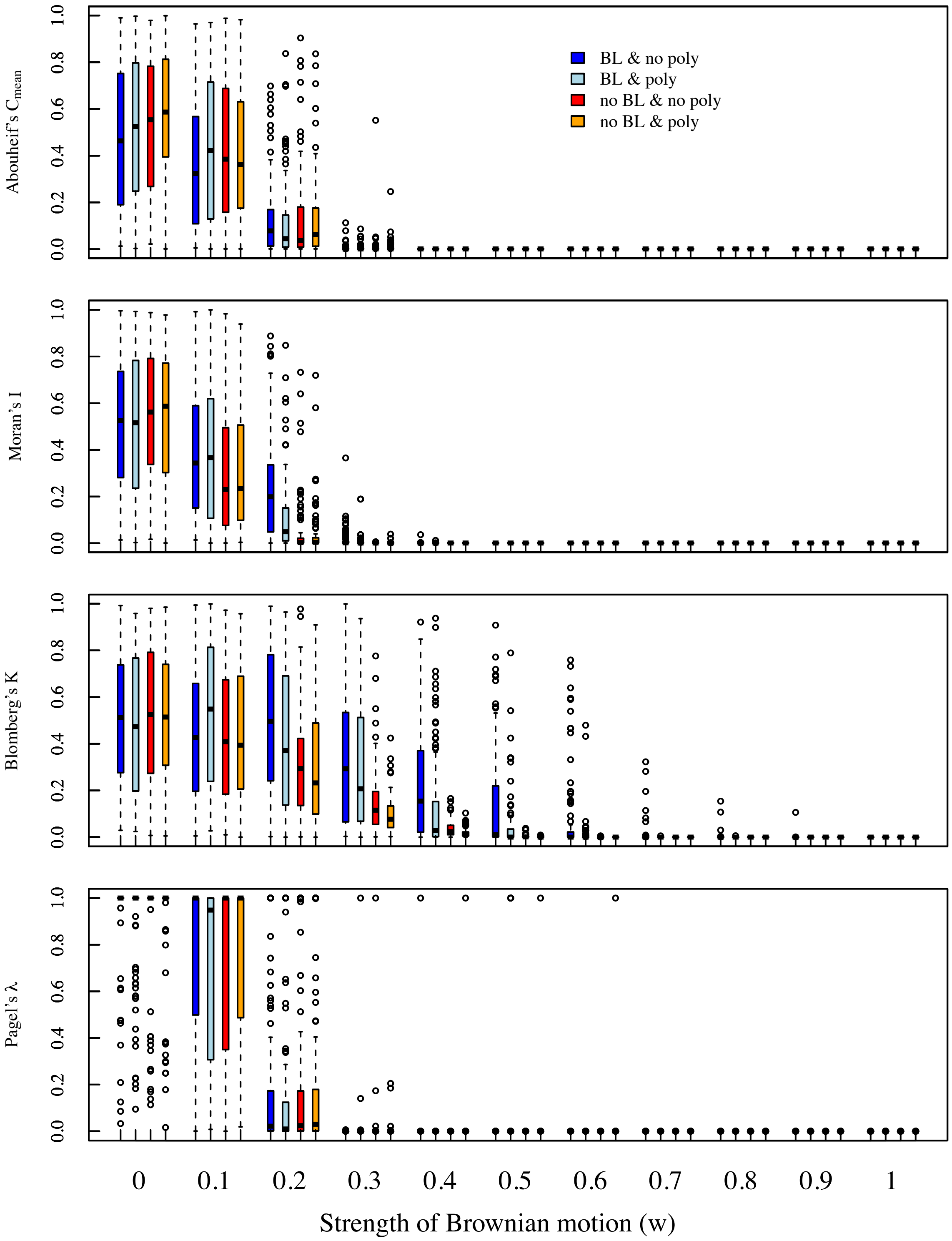

Figure A2

Response of phylogenetic signal tests (*p*-values for observed values given the null model distributions) to polytomies and branch length information (shown are scenarios for 500 species).

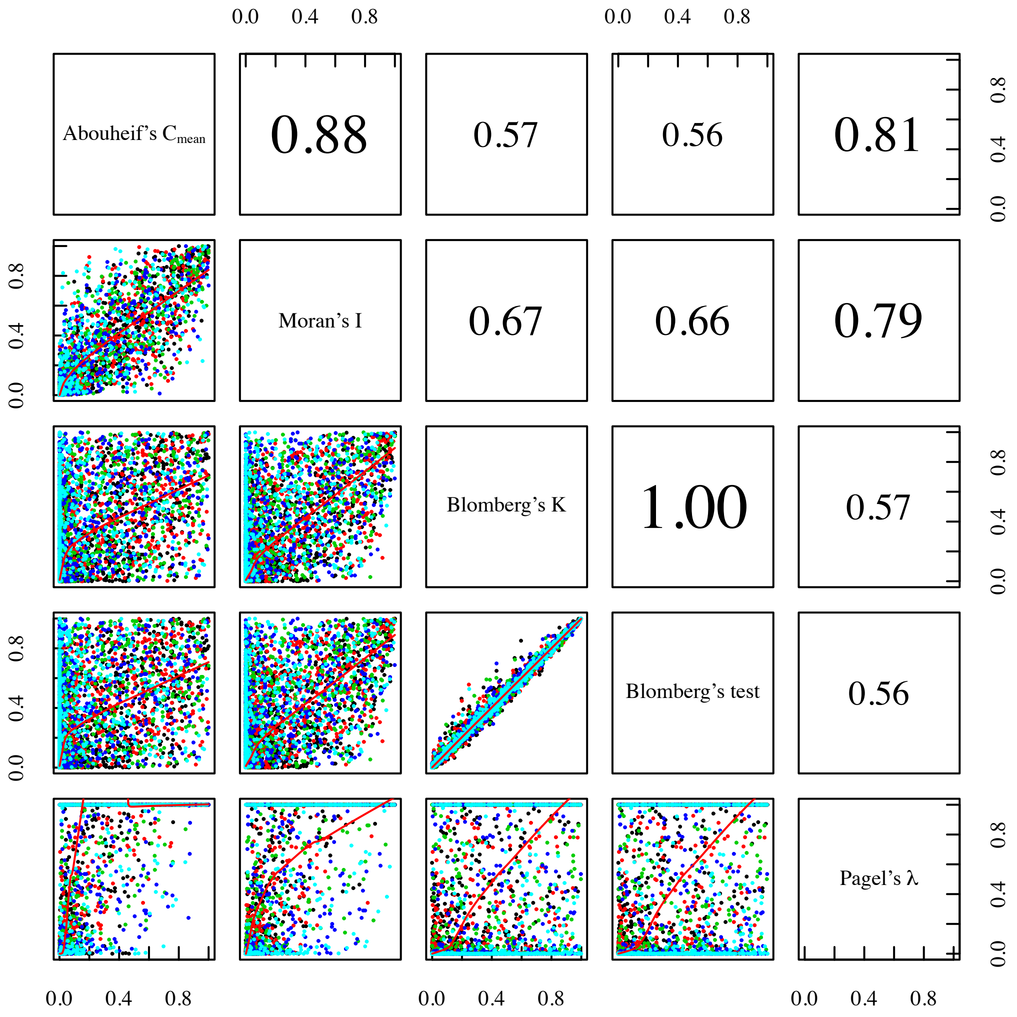

Figure A3

Correlation of phylogenetic signal tests (*p*-values for observed values given the null model distributions) for different N (black indicates 20, red 50, green 100, blue 250 and turquois 500 species). Shown are scenarios for all strengths of Brownian motion, with branch length information and no polytomies.

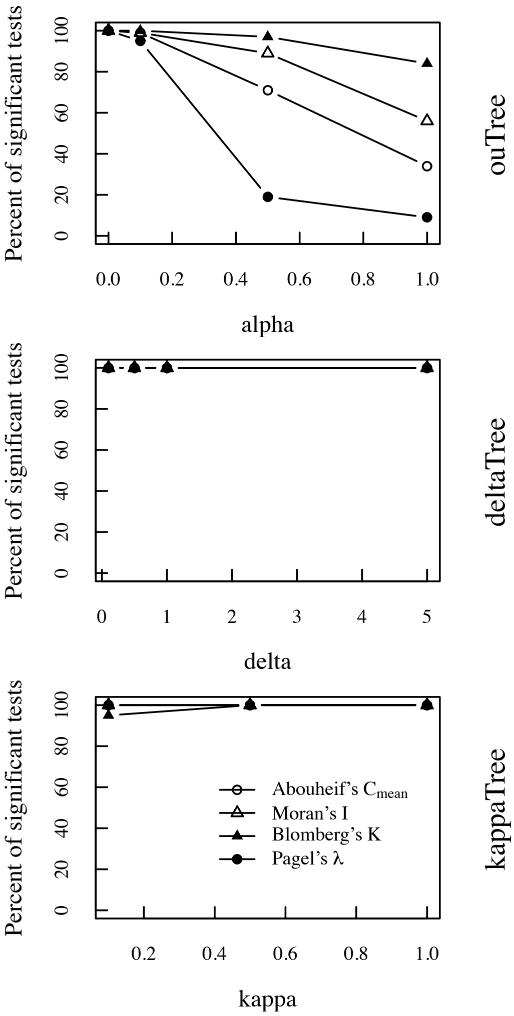

Figure A4

Response of phylogenetic signal tests to increasing values of the parameters for different tree transformations (shown are scenarios with 100 species, with branch length information and no polytomies). Figures refer to the rejection rate for the null hypothesis that there is no phylogenetic signal. OuTree corresponds to evolution under an Ornstein-Uhlenbeck model, i.e. a random-walk model with a central tendency with strength α (α = 0 is Brownian motion, BM); deltaTree simulates a slow-down or speed-up in the rate of character evolution through time (δ =1 is BM, δ >1 is speed-up, δ <1 is slow-down; kappaTree simulates "speciational" models (κ = 1 is BM, κ = 0 is a speciational model).

A2 Similarity of our simulations to a λ model of trait evolution

Pagel's λ describes the proportion of trait variance that can be attributed to Brownian motion. If we formulate the trait evolution model with the weighting factor w (w-model) as $y = w * x + (1\text{-}w) * x_{rand}$, where y is the final trait vector (*trait* in the main text), x is the trait vector under Brownian motion ($trait_{BM}$ in the main text) and x_{rand} the randomized trait vector ($trait_{rand}$ in the main text) then the expected value for Pagel's λ is var($w * x$) / var(y). From this follows (because x and x_{rand} are independent and have the same variance):

$\text{var}(y) = \text{var}(w * x) + \text{var}((1\text{-}w) * x_{rand}) = w^2 \text{ var}(x) + (1\text{-}w)^2 \text{ var}(x_{rand}) = \text{var}(x) \ (w^2 + (1\text{-}w)^2 \ )$

and if var(x) = 1, then

$\text{var}(w * x) / \text{var}(y) = w^2 / (w^2 + (1\text{-}w)^2 \ )$

Therefore the relationship between w and Pagel's λ is s-shaped (see also Fig. A5) and the w-model can be reformulated such that w is the expected value for the estimated values of Pagel's λ (λ -model): $y = w^{1/2} * x + (1\text{-}w)^{1/2} * x_{rand}$

The following R-code (major parts were provided by an anonymous reviewer) nicely visualizes that (1) using the w-model of trait evolution the relationship between w and Pagel’s λ (and between w and Blomberg’s K) is s-shaped (Fig. A5, left plots, see also e.g. Fig. 2 and 3), (2) that this relationship can be linearized if not w is plotted on the x-axis but $w^2/(w^2+(1\text{-}w)^2)$ instead (and in addition if not Blomberg’s K is plotted on the y-axis but $-1/K$, Fig. A5, left plots) and (3) that a λ-model of trait evolution results in a very good match of Pagel’s λ with mean w values (and in a linear relationship of w with $-1/K$, Fig. A5, right plots).

```
require(phytools)
require(geiger)
mean.lambda <- mean.K <- mean.lambda_l <- mean.K_l <- rep(0, 11)
w <- c(0:10/10)
for(i in 1:100){
  # simulate phylogenetic tree with 100 tips
  tree <- rescaleTree(drop.tip(birthdeath.tree(b=1, d=0,
    taxa.stop=101),"101"),1)
  x <- fastBM(tree) # trait vector with BM trait
  y <- sample(x) # trait vector with randomized trait
```

```
  names(y) <- names(x)
  for(j in 1:11){
    z <- w[j] * x + (1 - w[j]) * y # trait vector (w-model)
    mean.lambda[j] <- mean.lambda[j] + phylosig(tree, z,
       method="lambda")$lambda/100 # Pagel’s λ
    mean.K[j] <- mean.K[j] + phylosig(tree,z)/100 # Blomberg’s K
    z_l <- sqrt(w[j]) * x + sqrt(1 - w[j]) * y # trait vector (λ-model)
    mean.lambda_l[j] <- mean.lambda_l[j] + phylosig(tree, z_l,
       method="lambda")$lambda/100 # Pagel’s λ
    mean.K_l[j] <- mean.K_l[j] + phylosig(tree,z_l)/100 # Blomberg’s K
  }
}
tf_w <- w^2/(w^2+(1-w)^2) # transformed w
tf_K <- -1/mean.K + max(1/mean.K) # transformed K
```

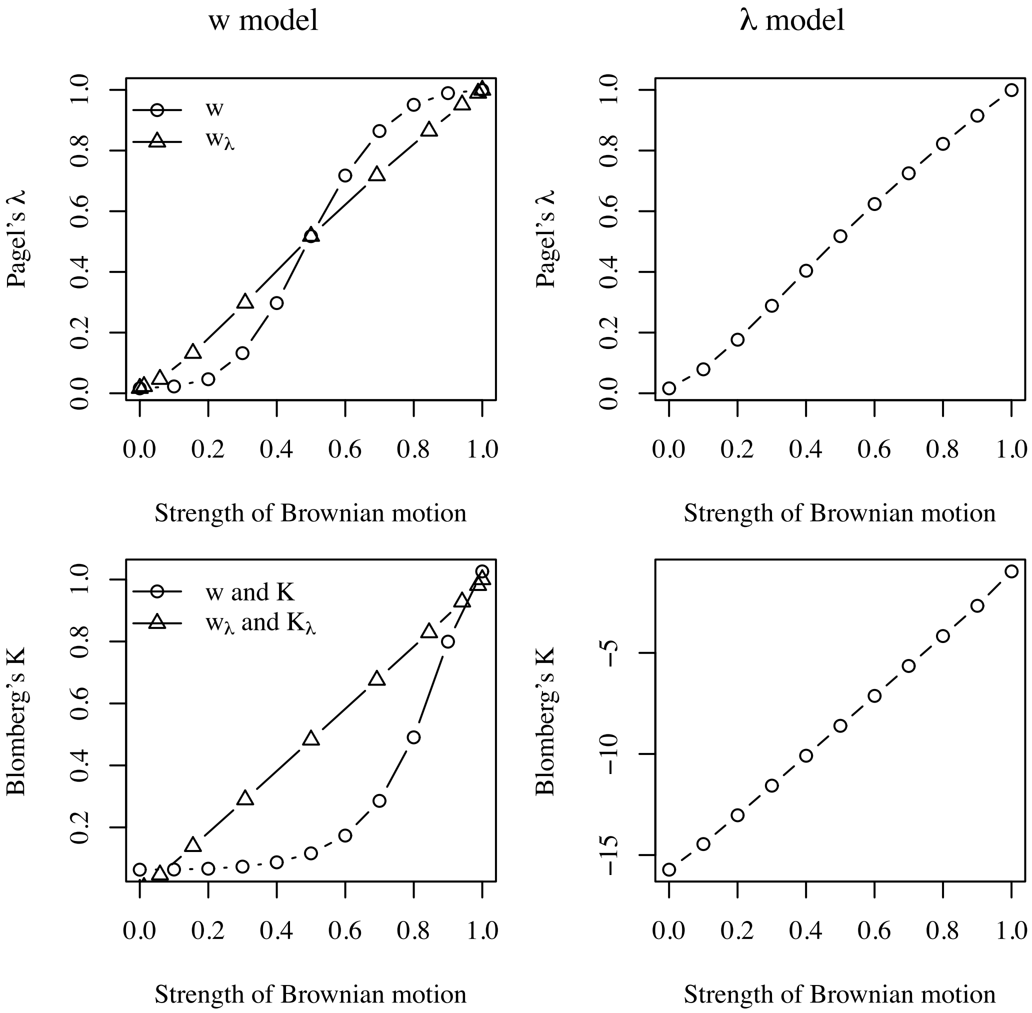

Figure A5

Comparison of phylogenetic signal values against increasing strength of Brownian motion for the model of trait evolution applied in this paper (*w* model, plots on the left) and a λ model of trait evolution (plots on the right). For the *w* model, the strength of trait evolution is linearly related to Pagel's λ only if it is described by a transformation of w, w_λ. The relationship with Blomberg's K requires the same transformation of w and in addition a transformation of K, K_λ (see Appendix A2 for details).

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