Title page

Manuscript title: How to define, use, and interpret Pagel's λ (lambda) in ecology and evolution

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Keywords: Comparative analysis, phylogeny, evolutionary correction, Brownian motion, heritability, Bayesian, hierarchical model, generalised least squares, univariate, multivariate.

Open research statement: No data were used or collected as part of this work.

1   Abstract

Pagel's λ (lambda) is a critical tool in ecology and evolution for describing trait evolution, imputing missing species' data, and generalising ecological relationships beyond their study system. Yet the interpretation of λ depends on context, and there are many misconceptions about metrics that are similar but not identical to λ. As an index of phylogenetic signal applied to continuous traits, λ typically (but not always) ranges between 0 and 1, and is a rate-independent measure of the degree to which closely-related species resemble one-another relative to a Brownian motion expectation. But this measure is biased by non-random species sampling—a common characteristic of ecological data—which also makes phylogenetic imputation of missing traits challenging. The λ estimated in regression models has little to do with the phylogenetic signal of measured traits and is better considered as either a statistical correction or a measure of the impact of unmeasured (latent) traits in the model. In other contexts, such as hierarchical models including intra-specific variation, λ is frequently confused with distinct metrics such as h^2. We show how confusion in defining and using λ can mislead our interpretation of ecological and evolutionary processes.

2   Introduction

Species traits are fundamental to our understanding of community assembly, the functioning of ecosystems, and how species might respond to environmental change (Bolnick et al., 2011; Foden et al., 2013; Violle et al., 2007). There is, therefore, large interest in modelling trait correlations, the interactions between traits, and in estimating trait lability. Because ecological interactions both shape and are shaped by the evolution of traits, integrating eco-evolutionary feedbacks operating over both short (Fussmann et al., 2007) and long (Cavender-Bares et al., 2009) timescales can help advance trait research. Reflecting this reality, these is now widespread application of phylogenetic comparative methods in ecology and global change research (Ackerly, 2009; Cavender-Bares et al., 2012; Edwards et al., 2007).

One of the most common uses of phylogeny in ecology is to detect and interpret patterns in species' traits. Phylogenetic signal—the tendency for closely related species to share similar trait values—violates statistical assumptions of independence in many ecological analyses and so requires statistical correction (Freckleton et al., 2002). Correcting for this non-independence was one of the first uses of phylogenetic comparative methods (Felsenstein, 1985). Perhaps one of the most widely estimated phylogenetic signal metrics is Pagel's λ (Pagel, 1999), a phylogenetic scaling parameter that describes how the shared evolutionary histories of species explain patterns of similarity observed in data. Often Pagel's λ (lambda) is implicitly treated as the only relevant phylogenetic metric, but it is actually the third of the three phylogenetic transformations introduced by Pagel (1999). The other Pagel transformations, δ and κ, represent alternative modes of evolution that capture shifts in evolutionary rates, either across the depth of the tree (δ) or at speciation events (κ), but λ is the more frequently used (Münkemüller et al., 2012).

Here we review the definition of Pagel's λ which, by virtue of being an algorithmic transformation, has different interpretations in different statistical contexts. We attempt to resolve some of the resulting confusion by considering its usage as an estimate of the phylogenetic signal in a single trait, including the impact of missing data and incomplete sampling in its estimation, as a scaling parameter estimated in classical trait regression, and in the emerging field of flexible hierarchical models of species' ecological responses to environmental change.

We highlight five key points: (1) when estimated on a single trait, λ measures whether trait evolution is consistent with Brownian motion, which is not the same as evolutionary rate or phylogenetic correlation. (2) Ecological assembly is non-random, and so estimates of signal in ecological communities should be treated with caution. (3) Imputing traits on the basis of phylogeny is fraught with uncertainty, even if taxonomic sampling is fair and random (which, unfortunately, it rarely is). (4) λ in Phylogenetic Generalised Least Squares models has essentially very little to do with the phylogenetic signal of the modelled traits, but is an important statistical correction and can provide insight into the broader drivers of trait relationships. (5)

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65 New hierarchical methods offer exciting opportunities to estimate the evolution of species'

66 ecological responses, but Pagel's λ cannot be estimated from variance ratios and thus is not the

67 same as heritability (h^2).

3 Defining Pagel's λ

69 It is remarkably difficult to pinpoint exactly when Pagel's λ was first defined, but the most

70 common citation is to Pagel (1999) where λ is discussed in detail (the original citation and

71 derivation of λ remain somewhat obscure). λ is broadly described as a multiplier of a phylogeny's

72 internal branch lengths, but is more precisely—and correctly—described as *a multiplier of the*

73 *off-diagonal elements of the phylogenetic variance-covariance matrix.* For example, in a

74 three-species phylogeny (as depicted in figure 1), the λ transformation is applied to the

75 phylogenetic variance-covariance matrix (V_{phy}) to produce a resulting variance-covariance matrix

76 (Σ) as follows:

$$V_{phy} = \begin{bmatrix} \sigma_1^2 & \sigma_{12} & \sigma_{1,3} \\ \sigma_{2,1} & \sigma_2^2 & \sigma_{2,3} \\ \sigma_{3,1} & \sigma_{3,2} & \sigma_3^2 \end{bmatrix} \tag{1}$$

$$\Sigma = \begin{bmatrix} \sigma_1^2 & \lambda \cdot \sigma_{12} & \lambda \cdot \sigma_{1,3} \\ \lambda \cdot \sigma_{2,1} & \sigma_2^2 & \lambda \cdot \sigma_{2,3} \\ \lambda \cdot \sigma_{3,1} & \lambda \cdot \sigma_{3,2} & \sigma_3^2 \end{bmatrix} \tag{2}$$

77 Where σ refers to (co)variances indexed by their subscripts, such that, for example, σ_1^2 reflects the

78 'diagonal' variance unique to the first species, and $\sigma_{1,2}$ the covariance shared by species 1 and 2.

79 The variances (the diagonals of Σ) are equal to the root-to-tip distances for each species on the

80 phylogeny and are unaltered by λ; the covariances reflect the shared branch-length between pairs

81 of species.

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λ was initially introduced to capture the degree of similarity among species as an index of phylogenetic signal in a measured trait: "*whether the phylogeny correctly predicts the patterns of covariance among species on a given trait*" (Pagel, 2002b). However, Pagel (2002a) also describes λ as a measure of the "*extent to which it is necessary when investigating trait evolution to take the phylogeny into account*". With the rapid expansion of phylogenetic comparative methods following Felsenstein's seminal paper on independent contrasts (1985), the latter usage has become widely adopted. Pagel's λ was subsequently incorporated into the phylogenetic regression, popularised in Phylogenetic Generalised Least Squares (PGLS; Freckleton et al., 2002) as implemented in the *R* (R Core Team, 2021) package '*caper*' (Orme et al., 2013).

Not all implementations or definitions of λ are the same: the *R* package *brms* (Bürkner, 2021), for example, defines it in terms of a variance ratio (equation 5; discussed in detail below). These varying definitions in part reflect the pace of development in the field of comparative methods, but also make it more difficult to compare estimates of λ. As we outline below, while it has been suggested that other formulations are equivalent, those equivalencies are, at best, controversial and, at worst, wrong; so we suggest avoiding such simplifications.

4   Describing the evolution of a single trait

Pagel's λ is frequently used to describe the extent to which species' trait values are correlated with phylogeny, whether past evolution has been slowed by some constraints, or whether a particular ecological force has impacted the evolutionary trajectory of the trait. In many cases these interpretations are misinformed.

Pagel's λ measures phylogenetic signal, and uses Brownian motion as its marker of that signal. While there are alternative approaches for quantifying and testing for phylogenetic signal, or the related concept of phylogenetic niche conservatism, we do not explore them here as they have already been extensively reviewed and debated elsewhere (*e.g.*, Blomberg et al., 2003; Diniz-Filho et al., 2012; Losos, 2008; Münkemüller et al., 2015; Münkemüller et al., 2012; Wiens

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107   et al., 2010).

108   When estimated for a single continuous trait on an ultrametric phylogeny with branch lengths

109   proportional to time and tips (species) terminating at the present, λ represents the degree to which

110   the phylogenetic distance between species corresponds to differences in their trait values (figure

111   1). Values of $\lambda = 0$ match to a white noise model of evolution and indicate no phylogenetic

112   structure in traits: species' phylogenetic relationships do not predict their trait similarities. This

113   can also be represented by a 'star' phylogeny. Values of $\lambda = 1.0$ correspond to traits matching the

114   assumptions of Brownian motion, in which trait evolution approximates a random ("drunkard's")

115   walk through trait space. Typically $\lambda = 1.0$ is interpreted as evidence of strong phylogenetic

116   conservatism in trait evolution, although the definition, and best measure of phylogenetic

117   conservatism has been a matter of debate (Losos, 2008; Münkemüller et al., 2015). Phylogenetic

118   signal and niche conservatism, however, are not the same (Losos, 2008; Wiens et al., 2010).

119   When $0 < \lambda < 1$, which is what we most commonly observe (we are unaware of a systematic

120   review of such values, but see Harmon et al., 2010; Pennell et al., 2015), species' traits appear

121   intermediate between white noise and Brownian motion models. In such intermediate cases, traits

122   are less similar amongst species than expected from their phylogenetic relationships under

123   assumptions of Brownian motion, but closely related species are more similar to each other than

124   expected by chance. λ is often sensitive to the presence of some degree of phylogenetic signal,

125   but its confidence intervals are sufficiently wide that λ estimates are rarely precise (Münkemüller

126   et al., 2012). A λ transformation is sometimes used in models of discrete (non-continuous) trait

127   evolution [*e.g.*, see *geiger::fitDiscrete* (Pennell et al., 2015)], where similar caveats apply to their

128   use, and alternative statistics have been proposed to better capture evolutionary signal in binary

129   traits (*e.g.*, Fritz & Purvis, 2010).

130   Values of $\lambda > 1.0$ have occasionally been reported, but are controversial (Revell et al., 2008).

131   While Pagel allowed λ to take such values, he explicitly stated that their interpretation was not

132   defined (Pagel, 2002b), and many modern fitting routines do not permit them (Orme et al., 2013;

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133 Pennell et al., 2014). Biologically, a λ greater than 1 represents a stretching of internal nodes

134 towards the present day (*i.e.*, the pendant edges of the phylogeny). Such a transformation

135 increases the evolutionary history that species share and so can be considered to be allowing for

136 more phylogenetic conservatism than a Brownian motion model across a phylogeny would

137 normally imply. Nonetheless, there is an upper bound to λ defined by the ratio of the total tree age

138 to the age of the youngest node (figure 1). Framed statistically, as λ is a transformation of the

139 phylogenetic covariance matrix, and—as no valid covariance matrix can have an off-diagonal

140 element larger than its diagonals—the upper bound of λ is determined by the ratios of the largest

141 off-diagonal and diagonal entries (see also Revell & Harmon, 2022). Empirically, at this λ

142 upper-limit the youngest node is brought to the present day and so no higher λ values can be

143 applied to the phylogeny because we measure traits in the present. Thus values > 1 are rarely fit

144 in practical terms because that upper limit is idiosyncratic to each phylogeny, complicating

145 comparison and interpretation among datasets.

146 Values of $\lambda < 0$ are not allowed, and would imply negative covariances such that trait values are

147 predicted to be more similar between less closely related species. Negative auto-correlation is a

148 regular feature of social networks (*e.g.* De Nooy, 2013), finance systems, (*e.g.* Koutmos, 1997)

149 and spatial data (*e.g.* Griffith & Arbia, 2010), but has been less explored as a model of trait

150 evolution. However, competitive character displacement and evolutionary convergence could

151 both, in theory, give rise to negative covariances (*i.e.*, traits that are over-dispersed relative to

152 Brownian expectations; Davies, Cooper, et al., 2012). Such negative correlation has been termed

153 'anti-signal', but we have not been able to find a definitive first reference for it in that context.

154 Nonetheless, negative patterns have been extensively studied in community phylogenetics

155 (termed 'phylogenetic over-dispersion') as a pattern (Webb et al., 2002) and in phylogenetic

156 generalised linear mixed modelling (Gallinat & Pearse, 2021; Ives & Helmus, 2011).

157 λ is a metric of the degree of fit with Brownian motion evolution, and so is independent of the rate

158 of evolution (Revell et al., 2008) which is included as a separate parameter (σ^2) in Brownian

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motion models. There are various metrics of the rate of trait evolution (*e.g.*, the Felsen; Ackerly, 2009), but λ is independent from them. We provide an illustration of this in the supplementary materials (see also (Revell et al., 2008)). That a trait is consistent with Brownian motion evolution does not mean either that the trait has evolved under strong selection or that the trait has evolved in the absence of selection (Revell et al., 2008). Brownian motion could be consistent with both the evolution of a fitness-neutral trait (Losos, 2008) or strong fluctuating selection (Revell et al., 2008), and there is little way to separate the two. Notably, standard models of Brownian motion do not contain a parameter to indicate the strength of selection, and the most commonly-used macro-evolutionary model that does (Ornstein-Uhlenbeck or OU models; Butler & King, 2004) is, itself, only contentiously mapped onto macro-evolutionary process (Cooper et al., 2016; Pearse et al., 2018).

5 The dangers of missing species and biased sampling

In estimating λ we assume the underlying phylogeny is known without error, which is almost certainly not the case. Fortunately, Pagel's λ is relatively robust to incomplete phylogenetic resolution and branch length errors (Molina-Venegas & Rodríguez, 2017), unlike some alternative metrics of phylogenetic signal such as Blomberg's K (Davies, Kraft, et al., 2012). Nonetheless, λ estimated on an incorrect tree topology will necessarily also be incorrect. Here, we highlight a more pernicious but under appreciated source of error: the choice of species for an analysis. In the supplementary materials, we give code examples of the impacts of these well-studied issues.

Pagel's λ was defined and derived under the expectation of a completely sampled, monophyletic dataset, and while λ tests are relatively robust to incomplete samples those samples should be representative of the true underlying phylogenetic distribution of trait values (Münkemüller et al., 2012). Because, Brownian motion is a noisy process it is possible, and indeed probable, that λ will differ when estimated on different species subsets (*e.g.* Rafferty & Nabity, 2017) even when the underlying evolutionary model is invariant. When species sets share ancestral lineages, each

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184 branch on the phylogeny can have only one true evolutionary history for a given trait; thus it

185 would be a mistake to interpret such differences as reflecting divergent evolutionary histories.

186 Estimates of λ derived from community data are even more challenging. Observed ecological

187 assemblages rarely, if ever, contain the entirety of a monophyletic lineage: indeed, most

188 ecological processes result in a non-random subset of species (often biased by ecological filtering

189 on the traits of interest themselves). Differences in λ estimated from phylogenetically overlapping

190 species sets might provide information on the process of community assembly (Prinzing et al.,

191 2021) or reveal environment-by-trait interactions for spatially structured data (*e.g.* Davies et al.,

192 2013). But non-random, ecologically filtered assemblages would not be expected to give reliable

193 insight into the broader evolutionary forces describing trait evolution across the entire clade.

6 Phylogenetic imputation of missing trait values

195 When measured traits on a species set exhibit strong phylogenetic signal, it can be tempting to use

196 phylogeny to impute trait values for unsampled species (Bruggeman et al., 2009). Phylogenetic

197 imputation provides an approach for gap-filling traits datasets without the need for expensive and

198 time consuming field work and trait measurement (Swenson, 2014). However, high λ in measured

199 traits is insufficient to ensure high accuracy in imputed data, and the noisiness of the Brownian

200 motion process makes predictions for species with few close-relatives particularly unreliable even

201 for traits showing strong evolutionary conservatism (Molina-Venegas et al., 2018). In some cases,

202 imputed values have been shown to be indistinct from noise (Molina-Venegas et al., 2023).

203 Nonetheless, particularly when combined with correlated trait data, phylogenetically informed

204 models can provide powerful approaches for interpolating missing values (Debastiani et al., 2021;

205 Penone et al., 2014) and should be preferred over non-phylogenetic models. The simplest solution

206 to handling uncertainty in imputed values is to ensure that errors associated with trait imputations

207 are propagated forward into subsequent analyses. This includes both the uncertainty from the

208 Brownian motion parameter (σ^2) and its impact on the standard error of the estimate, as well as

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209 the fit of the Brownian motion model itself (*i.e.*, model uncertainty).

7   Regressing two, or more, traits against one-another

211 Ecology has long been interested in trait correlations, using regression models to understand how

212 they relate to each other. In the 1990s and early 2000s there was great debate over the importance

213 of phylogeny in the regression of traits, especially as they relate to ecology (Harvey et al., 1995;

214 Westoby et al., 1995), and that debate has somewhat reopened recently (Uyeda et al., 2018;

215 Westoby et al., in press). While our purpose here is not to rehash that debate, a fair summary

216 would be that if we are interested in generalising relationships we explore to other species and/or

217 ecosystems, then an evolutionarily (phylogenetically) informed analysis is required to account for

218 species' non-independent evolution (Felsenstein, 1985; Harvey, Pagel, et al., 1991).

219 The development of phylogenetic comparative methods advanced rapidly over the 1990s and

220 2000s, with Phylogenetic Generalised Least Squares (PGLS; Freckleton et al., 2002), a

221 generalisation of Felsenstein's Phylogenetic Independent Contrasts (Felsenstein, 1985), now

222 commonly employed to regress traits across species. These methods can reveal that observed trait

223 correlations are the result of shared evolutionary history: this does not negate the obvious

224 presence of a correlation, but rather suggests that the correlation may result from shared historical

225 accident. To interpret λ in PGLS, we must first understand how the model is fit (which is detailed

226 in Freckleton et al., 2002). There is no simple equation that will report the maximum likelihood λ

227 value; instead, the model must be fit by maximising the likelihood (L) of the observed data given

228 different model coefficients (including λ).

229 PGLS is a variant of Generalised Least Squares (GLS) and, as in all GLS models, the

230 log-likelihood (L) function is:

$$L \propto -log(\sigma^2) - \frac{1}{2}log(|\Sigma|) - \frac{1}{2\sigma^2}(\mathbf{y} - \mathbf{X}\beta)'\Sigma^{-1}(\mathbf{y} - \mathbf{X}\beta) \tag{3}$$

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231 Where all terms are as already defined save the response variable (trait; $\mathbf{y}$), an explanatory

232 variable (trait(s); $\mathbf{X}$), the model coefficients (β), and the variance (σ^2; note that this is strongly

233 linked to the Brownian motion definition in equation 2). PGLS is different from GLS when

234 estimating λ only in that Σ is as defined in equation 2: its popularity and beauty stems from being

235 able to make use of the existing body of statistical theory about GLS.

236 There is some confusion about what λ estimates in PGLS (see Uyeda et al., 2018, for an excellent

237 discussion), perhaps in part because λ does not appear in the likelihood function (equation 3) but

238 rather is implicit in the definition of Σ (itself defined in equation 2). Importantly, the λ estimated

239 in a PGLS is *not* the phylogenetic signal of any of the traits involved in the regression. It is not

240 only possible, but common, for two traits with phylogenetic signal to return an estimated λ of 0

241 when regressed against one another in PGLS (in the supplementary materials we give a

242 demonstration of this surprising, but well-established, property). This is because a PGLS fits λ

243 not just to the transformed matrix Σ but also to the residuals (species-specific errors; $\mathbf{y} - \mathbf{X}\beta$ in

244 equation 3) in the model. However, PGLS can be used to estimate the phylogenetic signal of a

245 trait if (and only if) the trait of interest is the response variable in the regression and the sole

246 explanatory variable is the intercept. In this special case the residuals of the PGLS are equal to the

247 variation in the response variable, and so the λ reported by a PGLS is the phylogenetic signal in

248 that trait and can be interpreted as such.

249 One way to interpret PGLS is that it allows the phylogeny to capture some putative latent trait that

250 affects the relationship between the directly modelled traits, and PGLS reveals the phylogenetic

251 patterning to that latent trait. This latent trait may enhance or mask the estimated statistical

252 relationship between the modelled variables that would be apparent in the absence of this

253 confounding evolutionary pattern.

254 Phylogenetic regression (*sensu* Grafen, 1989) and PGLS are not the only ways to quantify

255 multi-trait evolutionary information. Phylogenetically-informed versions of dimension-reduction

256 techniques, such as ordination or principal component analysis (PCA), that leverage λ also exist.

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In cases where the goal is to identify general patterns and groupings of traits (and there is no particular response variable), then phylogenetic redundancy analysis (RDA) and PCA (Revell & Harrison, 2008) are useful methods. While we do not consider those approaches here, we emphasise that λ estimated in a novel context (*e.g.*, a PCA), will require careful reassessment, and may not always be interpreted analogously to λ in a PGLS, even if fit similarly as a transformation of the phylogenetic variance-covariance matrix.

8   Hierarchical models

With modern approaches (*e.g.* Hadfield et al., 2014; Ives & Helmus, 2011), and in particular the advent of flexible Bayesian methods (Uyeda & Harmon, 2014), we are no longer restricted to fitting models where phylogenetic information, such as λ, can only be accounted for in the residual error structure. These new approaches allow us to answer questions about how species' responses to environment and other species have evolved, and are an exciting avenue for eco-evolutionary research (Gallinat & Pearse, 2021). There is a need for caution, however; as there are myriad links and generalisations that bind different hierarchical approaches it can be challenging to understand when they apply to λ.

The implementation of such hierarchical models is described elsewhere in greater detail (*e.g.* Gallinat & Pearse, 2021; Ives & Helmus, 2011), but in brief: hierarchical models can be fit where species' coefficients (*e.g.*, environmental responses or interaction coefficients) are drawn from distributions parameterised by phylogenetic covariance matrices that are, themselves, scaled by λ. We expand on the approach described by Ives (2019) to define such a covariance matrix (Σ), specifically:

$$\Sigma = \sigma^2 \lambda V_{phy} + \sigma^2 (1 - \lambda)\mathbf{I} \tag{4}$$

Where σ^2 is the Brownian motion rate parameter and $\mathbf{I}$ the identity matrix (a matrix where the

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279 diagonals are all 1 and the off-diagonals are all 0). Equation 4 is essentially an algebraic

280 re-arrangement of equations 1 and 2 to allow for a more efficient estimation of Σ that makes

281 separating its phylogenetic (V_{phy}) and non-phylogenetic ($\mathbf{I}$) components more straightforward. In

282 practice models may not be fit with precisely this formulation, more often employing some form

283 of algorithmic shorthand or Cholesky decomposition to speed estimation, but the fundamentals

284 are the same (Ho & Ane, 2014; Pearse et al., 2015).

285 It is possible and conceptually appealing to partition variance into phylogenetic and

286 non-phylogenetic components, and thus derive the ratio of the phylogenetic component to the

287 total variance, heritability (h^2; see Hadfield & Nakagawa, 2010; Lynch, 1991):

$$h^2 = \frac{\sigma_p^2}{\sigma_p^2 + \sigma_e^2} \tag{5}$$

288 Where σ_p^2 is a variance multiplied by a phylogenetic variance-covariance matrix (akin to V_{phy} in

289 equation 4) during model fitting, and σ_e^2 is the residual error variance across the entire model.

290 While precise definitions for the terms within this equation depend on context, the spirit of it is

291 always a variance ratio: variance associated with phylogeny (σ_p^2) compared to the total variance in

292 the model ($\sigma_p^2 + \sigma_e^2$).

293 Confusion can arise when comparing Pagel's λ to such estimates of phylogenetic heritability from

294 hierarchical models, and when trying to find equivalencies among them. There has been debate on

295 the exact equivalency of λ and h^2, since it is not possible to fit the two formulations above

296 (equations 4 and 5) simultaneously, yet phylogenetic signal seems, intuitively, similar to the

297 amount of variation in data explained by phylogeny. This intuition is almost always incorrect,

298 however. Housworth et al. (2004) suggest the two metrics are mathematically equivalent; this

299 cannot be the case since, as Freckleton et al. (2002) highlight, h^2 is bounded between 0 and 1, but

300 λ is not a ratio and can take values >1 as we discuss above. Confusingly, under strict assumptions

301 of Brownian motion evolution, both λ and h^2 are expected to be 1, and both are expected to be 0

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302 for traits in the absence of phylogenetic structure (Freckleton et al., 2002). It thus seems

303 reasonable to expect that for intermediary cases h^2 and λ will also be similar, but this is not

304 necessarily the case; those who, like us, have followed too closely advice from standard statistical

305 software (*e.g.*, Bürkner, 2021) need not panic, but simply recognise these different model

306 formulations and carefully report the metrics calculated.

307 The variance partitioning approach has some limitations as it suggests separating coefficients that

308 may be better represented as intertwined. For example, take a model of the form:

$$y_i \sim normal(a + b, \sigma_e^2) \tag{6}$$

$$a \sim normal(\alpha, V_{phy} \cdot \sigma_p^2) \tag{7}$$

$$b \sim normal(\beta, \sigma_n^2) \tag{8}$$

309 Where y_i are observations of some trait (y) across species (indexed by i) drawn from a normal

310 distribution centred according to phylogenetic (a) and non-phylogenetic (b) components with

311 some overall error variance (σ_e^2). The species-level estimates are themselves drawn from a normal

312 distribution centred at some mean (α or β) with a variance informed by a phylogenetic

313 variance-covariance matrix (V_{phy}) with some estimated phylogenetic variance (σ_p^2) or

314 independently (σ_n^2). This kind of model (although most often used with replicate measurements of

315 species and with additional explanatory variables) is advocated for in some ecological contexts

316 (Bürkner, 2021), likely in part because PGLS is not well formulated to accommodate multiple

317 observations across species (but see Freckleton & Rees, 2019; Joly et al., 2019). In such cases, h^2

318 has been defined incorporating all three variance terms:

$$h^2 = \frac{\sigma_p^2}{\sigma_e^2 + \sigma_p^2 + \sigma_n^2} \tag{9}$$

319 There are two problems with such a formulation. First, even if the original Lynch (1991)

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320 formulation maps onto Pagel's λ equation 9, and the many diverse models it allows, it has not

321 been formally confirmed to do so. Second, this formulation is statistically inefficient and

322 potentially biased because it is co-estimating variance associated with species using two separate

323 distributions (Bafumi & Gelman, 2007). The phylogenetic and non-phylogenetic terms are, in

324 effect, competing for variance when they should be jointly fitting it.

325 The development of new statistical models that include phylogeny is exciting. Advances in model

326 fitting and speed may allow for greater flexibility in estimating the evolution of species'

327 environmental responses and interactions (Gallinat & Pearse, 2021) and allowing for interactions

328 with latent traits, represented by the phylogeny (Morales-Castilla et al., in review). However,

329 along with such advances is a need to better understand the equivalencies of parameters estimated

330 under alternative model formulations.

331 Lynch (1991) offered conceptual simplicity by estimating the fraction of variation that is

332 explained by phylogeny. Pagel's λ (1999) offers statistically efficiency, and maps nicely onto

333 well-studied concepts such as Brownian motion evolution. Here we suggest an approach that

334 combines the two: using a pooling metric, ω (named following Gelman & Pardoe, 2006), that

335 captures the variance in model fit attributable to species-specific variation using Pagel's λ

336 transformation:

$$\omega = \frac{\sigma^2 \lambda V_{phy} + \sigma^2(1-\lambda)\mathbf{I}}{\sigma^2 \lambda V_{phy} + \sigma^2(1-\lambda)\mathbf{I} + \sigma_e^2} \tag{10}$$

337 Where all other terms are as defined in equation 4 and above. This provides flexibility (additional

338 hierarchical terms could be added and then included in the denominator) and speed of estimation

339 (since all variance-covariance matrices would be estimated as outlined above in reference to

340 equation 4). We suggest such a metric would be of particular use in forecasting responses in

341 under-studied species, for which we may have phylogenetic information but limited ecological

342 observations.

15

9   Summary

Pagel's λ (lambda) is useful for measuring pattern in evolutionary process, and helps generalise findings beyond a particular ecological study system. We have discussed how λ is estimated, and the common pitfalls in its application and reporting. Specifically:

- λ is (usually) a number between 0 and 1 that measures phylogenetic signal, but care must be taken as it can exceed 1 and there are many different definitions of phylogenetic signal.

- When estimating signal in individual traits, λ is sensitive but imprecise, and non-random taxon sampling—common in ecology—can bias estimates.

- λ is independent of evolutionary rate, and the interpretation of differences in λ estimated on phylogenetically overlapping taxon sets is not straightforward.

- High λ is likely not a useful index of adaptive constraints to global change as it integrates across (macro)evolutionary processes operating over long timescales (often millions of years), and does not necessarily provide information on constraints to adaptation over short timescales.

- High λ is necessary but not sufficient for successful phylogenetic imputation of missing trait data.

- In classical regression modelling, λ allows us to account for latent traits that covary with phylogeny and potential statistical confounds, but it is not a panacea and is informative on the residual (latent) variation only.

- When estimated in a phylogenetic least squares regression, λ can be zero even when measured traits are phylogenetically structured, because λ is estimated using the residual errors.

- Hierarchical models are powerful tools to study the evolutionary history of ecological processes, but the foundational definitions and linkages among statistical approaches

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367   complicate interpretation of λ, and different derivations are not always interchangeable.

368   • Estimates of heritability (h^2) derived from hierarchical models are often similar to Pagel's

369   λ, but are only equivalent to λ under a set of very limited situations.

370   • As we move forward with a new era of complex, flexible modelling, we must be careful to

371   report precisely what we have calculated in our models, and not assume that equivalencies

372   in one domain apply to another.

Acknowledgements

References

376 Ackerly, D. D. (2009). Phylogenetic methods in ecology. *eLS*.

377 Bafumi, J., & Gelman, A. (2007). Fitting multilevel models when predictors and group effects

378   correlate. *Available at SSRN 1010095*.

379 Blomberg, S. P., Garland Jr, T., & Ives, A. R. (2003). Testing for phylogenetic signal in

380   comparative data: Behavioral traits are more labile. *Evolution*, *57*(4), 717–745.

381 Bolnick, D. I., Amarasekare, P., Araújo, M. S., Bürger, R., Levine, J. M., Novak, M.,

382   Rudolf, V. H., Schreiber, S. J., Urban, M. C., & Vasseur, D. A. (2011). Why intraspecific

383   trait variation matters in community ecology. *Trends in Ecology & Evolution*, *26*(4),

384   183–192.

385 Bruggeman, J., Heringa, J., & Brandt, B. W. (2009). Phylopars: Estimation of missing parameter

386   values using phylogeny. *Nucleic acids research*, *37*(suppl_2), W179–W184.

387 Bürkner, P.-C. (2021). Bayesian item response modeling in R with brms and Stan. *Journal of*

388   *Statistical Software*, *100*(5), 1–54.

Butler, M. A., & King, A. A. (2004). Phylogenetic comparative analysis: A modeling approach for adaptive evolution. *The American Naturalist*, *164*(6), 683–695.

Cavender-Bares, J., Ackerly, D. D., & Kozak, K. H. (2012). Integrating ecology and phylogenetics: The footprint of history in modern-day communities. *Ecology*, S1–S3.

Cavender-Bares, J., Kozak, K. H., Fine, P. V., & Kembel, S. W. (2009). The merging of community ecology and phylogenetic biology. *Ecology letters*, *12*(7), 693–715.

Cooper, N., Thomas, G. H., & FitzJohn, R. G. (2016). Shedding light on the 'dark side' of phylogenetic comparative methods. *Methods in Ecology and Evolution*, *7*(6), 693–699.

Davies, T. J., Cooper, N., Diniz-Filho, J. A. F., Thomas, G. H., & Meiri, S. (2012). Using phylogenetic trees to test for character displacement: A model and an example from a desert mammal community. *Ecology*, *93*(sp8), S44–S51.

Davies, T. J., Kraft, N. J., Salamin, N., & Wolkovich, E. M. (2012). Incompletely resolved phylogenetic trees inflate estimates of phylogenetic conservatism. *Ecology*, *93*(2), 242–247.

Davies, T. J., Wolkovich, E. M., Kraft, N. J., Salamin, N., Allen, J. M., Ault, T. R., Betancourt, J. L., Bolmgren, K., Cleland, E. E., Cook, B. I., et al. (2013). Phylogenetic conservatism in plant phenology. *Journal of ecology*, *101*(6), 1520–1530.

De Nooy, W. (2013). Communication in natural resource management: Agreement between and disagreement within stakeholder groups. *Ecology and Society*, *18*(2).

Debastiani, V. J., Bastazini, V. A., & Pillar, V. D. (2021). Using phylogenetic information to impute missing functional trait values in ecological databases. *Ecological Informatics*, *63*, 101315.

Diniz-Filho, J. A. F., Bini, L. M., Rangel, T. F., Morales-Castilla, I., Olalla-Tárraga, M. Á., Rodríguez, M. Á., & Hawkins, B. A. (2012). On the selection of phylogenetic eigenvectors for ecological analyses. *Ecography*, *35*(3), 239–249.

Edwards, E. J., Still, C. J., & Donoghue, M. J. (2007). The relevance of phylogeny to studies of global change. *Trends in Ecology & Evolution*, *22*(5), 243–249.

18

Felsenstein, J. (1985). Phylogenies and the comparative method. *The American Naturalist*, *125*(1), 1–15.

Foden, W. B., Butchart, S. H., Stuart, S. N., Vié, J.-C., Akçakaya, H. R., Angulo, A., DeVantier, L. M., Gutsche, A., Turak, E., Cao, L., et al. (2013). Identifying the world's most climate change vulnerable species: A systematic trait-based assessment of all birds, amphibians and corals. *PloS one*, *8*(6), e65427.

Freckleton, R. P., Harvey, P. H., & Pagel, M. (2002). Phylogenetic analysis and comparative data: A test and review of evidence. *The American Naturalist*, *160*(6), 712–726.

Freckleton, R. P., & Rees, M. (2019). Comparative analysis of experimental data. *Methods in Ecology and Evolution*, *10*(8), 1308–1321.

Fritz, S. A., & Purvis, A. (2010). Selectivity in mammalian extinction risk and threat types: A new measure of phylogenetic signal strength in binary traits. *Conservation Biology*, *24*(4), 1042–1051.

Fussmann, G. F., Loreau, M., & Abrams, P. A. (2007). Eco-evolutionary dynamics of communities and ecosystems. *Functional ecology*, 465–477.

Gallinat, A. S., & Pearse, W. D. (2021). Phylogenetic generalized linear mixed modeling presents novel opportunities for eco-evolutionary synthesis. *Oikos*, *130*(5), 669–679.

Gelman, A., & Pardoe, I. (2006). Bayesian measures of explained variance and pooling in multilevel (hierarchical) models. *Technometrics*, *48*(2), 241–251.

Grafen, A. (1989). The phylogenetic regression. *Philosophical Transactions of the Royal Society of London. B, Biological Sciences*, *326*(1233), 119–157.

Griffith, D. A., & Arbia, G. (2010). Detecting negative spatial autocorrelation in georeferenced random variables. *International Journal of Geographical Information Science*, *24*(3), 417–437.

Hadfield, J. D., Krasnov, B. R., Poulin, R., & Nakagawa, S. (2014). A tale of two phylogenies: Comparative analyses of ecological interactions. *The American Naturalist*, *183*(2), 174–187.

19

443 Hadfield, J., & Nakagawa, S. (2010). General quantitative genetic methods for comparative

444   biology: Phylogenies, taxonomies and multi-trait models for continuous and categorical

445   characters. *Journal of evolutionary biology*, *23*(3), 494–508.

446 Harmon, L. J., Losos, J. B., Jonathan Davies, T., Gillespie, R. G., Gittleman, J. L.,

447   Bryan Jennings, W., Kozak, K. H., McPeek, M. A., Moreno-Roark, F., Near, T. J., et al.

448   (2010). Early bursts of body size and shape evolution are rare in comparative data.

449   *Evolution*, *64*(8), 2385–2396.

450 Harvey, P. H., Pagel, M. D., et al. (1991). *The comparative method in evolutionary biology*

451   (Vol. 239). Oxford university press Oxford.

452 Harvey, P. H., Read, A. F., & Nee, S. (1995). Why ecologists need to be phylogenetically

453   challenged. *Journal of Ecology*, *83*(3), 535–536.

454 Ho, L. S. T., & Ane, C. (2014). A linear-time algorithm for gaussian and non-gaussian trait

455   evolution models. *Systematic Biology*, *63*, 397–408.

456 Housworth, E. A., Martins, E. P., & Lynch, M. (2004). The phylogenetic mixed model. *The*

457   *American Naturalist*, *163*(1), 84–96.

458 Ives, A. R. (2019). R s for correlated data: Phylogenetic models, lmms, and glmms. *Systematic*

459   *Biology*, *68*(2), 234–251.

460 Ives, A. R., & Helmus, M. R. (2011). Generalized linear mixed models for phylogenetic analyses

461   of community structure. *Ecological Monographs*, *81*(3), 511–525.

462 Joly, S., Flynn, D. F., & Wolkovich, E. M. (2019). On the importance of accounting for

463   intraspecific genomic relatedness in multi-species studies. *Methods in Ecology and*

464   *Evolution*, *10*(7), 994–1001.

465 Koutmos, G. (1997). Feedback trading and the autocorrelation pattern of stock returns: Further

466   empirical evidence. *Journal of international money and finance*, *16*(4), 625–636.

467 Losos, J. B. (2008). Phylogenetic niche conservatism, phylogenetic signal and the relationship

468   between phylogenetic relatedness and ecological similarity among species. *Ecology*

469   *Letters*, *11*(10), 995–1003.

Lynch, M. (1991). Methods for the analysis of comparative data in evolutionary biology. *Evolution*, *45*(5), 1065–1080.

Molina-Venegas, R., Morales-Castilla, I., & Rodríguez, M. Á. (2023). Unreliable prediction of b-vitamin source species. *Nature Plants*, *9*(1), 31–33.

Molina-Venegas, R., Moreno-Saiz, J. C., Castro Parga, I., Davies, T. J., Peres-Neto, P. R., & Rodríguez, M. Á. (2018). Assessing among-lineage variability in phylogenetic imputation of functional trait datasets. *Ecography*, *41*(10), 1740–1749.

Molina-Venegas, R., & Rodríguez, M. Á. (2017). Revisiting phylogenetic signal; strong or negligible impacts of polytomies and branch length information? *BMC Evolutionary Biology*, *17*, 1–10.

Morales-Castilla, I., Davies, T., Legault, G., Buonaiuto, D., Chamberlain, C., Ettinger, A., Garner, M., Jones, F., Loughnan, D., Pearse, W., Sodhi, D., & Wolkovich, E. (in review). Phylogenetic estimates of species-level phenology improve ecological forecasting. *Nature Climate Change*, *0*, 0.

Münkemüller, T., Boucher, F. C., Thuiller, W., & Lavergne, S. (2015). Phylogenetic niche conservatism–common pitfalls and ways forward. *Functional Ecology*, *29*(5), 627–639.

Münkemüller, T., Lavergne, S., Bzeznik, B., Dray, S., Jombart, T., Schiffers, K., & Thuiller, W. (2012). How to measure and test phylogenetic signal. *Methods in Ecology and Evolution*, *3*(4), 743–756.

Orme, D., Freckleton, R., Thomas, G., Petzoldt, T., Fritz, S., Isaac, N., & Pearse, W. (2013). The caper package: Comparative analysis of phylogenetics and evolution in r. *R package version*, *5*(2), 1–36.

Pagel, M. (1999). Inferring the historical patterns of biological evolution. *Nature*, *401*(6756), 877–884.

Pagel, M. (2002a). Modelling the evolution of continuously varying characters on phylogenetic trees. *Morphology, shape and phylogeny*, *269*, 286.

Pagel, M. (2002b, January 23). *User's manual for continuous*. University of Reading.

Pearse, W. D., Barbosa, A. M., Fritz, S. A., Keith, S. A., Harmon, L. J., Harte, J., Silvestro, D., Xiao, X., & Davies, T. J. (2018). Building up biogeography: Pattern to process. *Journal of Biogeography*, *45*(6), 1223–1230.

Pearse, W. D., Cadotte, M. W., Cavender-Bares, J., Ives, A. R., Tucker, C. M., Walker, S. C., & Helmus, M. R. (2015). Pez: Phylogenetics for the environmental sciences. *Bioinformatics*, *31*(17), 2888–2890.

Pennell, M. W., Eastman, J. M., Slater, G. J., Brown, J. W., Uyeda, J. C., FitzJohn, R. G., Alfaro, M. E., & Harmon, L. J. (2014). Geiger v2. 0: An expanded suite of methods for fitting macroevolutionary models to phylogenetic trees. *Bioinformatics*, *30*(15), 2216–2218.

Pennell, M. W., FitzJohn, R. G., Cornwell, W. K., & Harmon, L. J. (2015). Model adequacy and the macroevolution of angiosperm functional traits. *The American Naturalist*, *186*(2), E33–E50.

Penone, C., Davidson, A. D., Shoemaker, K. T., Di Marco, M., Rondinini, C., Brooks, T. M., Young, B. E., Graham, C. H., & Costa, G. C. (2014). Imputation of missing data in life-history trait datasets: Which approach performs the best? *Methods in Ecology and Evolution*, *5*(9), 961–970.

Prinzing, A., Pavoine, S., Jactel, H., Hortal, J., Hennekens, S. M., Ozinga, W. A., Bartish, I. V., Helmus, M. R., Kühn, I., Moen, D. S., et al. (2021). Disturbed habitats locally reduce the signal of deep evolutionary history in functional traits of plants. *New Phytologist*, *232*(4), 1849–1862.

R Core Team. (2021). *R: A language and environment for statistical computing*. R Foundation for Statistical Computing. Vienna, Austria.

Rafferty, N. E., & Nabity, P. D. (2017). A global test for phylogenetic signal in shifts in flowering time under climate change. *Journal of Ecology*, *105*(3), 627–633.

Revell, L. J., & Harmon, L. J. (2022). *Phylogenetic comparative methods in r*. Princeton University Press.

22

Revell, L. J., Harmon, L. J., & Collar, D. C. (2008). Phylogenetic signal, evolutionary process, and rate. *Systematic Biology*, *57*(4), 591–601.

Revell, L. J., & Harrison, A. S. (2008). Pcca: A program for phylogenetic canonical correlation analysis. *Bioinformatics*, *24*(7), 1018–1020.

Swenson, N. G. (2014). Phylogenetic imputation of plant functional trait databases. *Ecography*, *37*(2), 105–110.

Uyeda, J. C., & Harmon, L. J. (2014). A novel bayesian method for inferring and interpreting the dynamics of adaptive landscapes from phylogenetic comparative data. *Systematic Biology*, *63*(6), 902–918.

Uyeda, J. C., Zenil-Ferguson, R., & Pennell, M. W. (2018). Rethinking phylogenetic comparative methods. *Systematic Biology*, *67*(6), 1091–1109.

Violle, C., Navas, M.-L., Vile, D., Kazakou, E., Fortunel, C., Hummel, I., & Garnier, E. (2007). Let the concept of trait be functional! *Oikos*, *116*(5), 882–892.

Webb, C. O., Ackerly, D. D., McPeek, M. A., & Donoghue, M. J. (2002). Phylogenies and community ecology. *Annual review of ecology and systematics*, *33*(1), 475–505.

Westoby, M., Leishman, M. R., & Lord, J. M. (1995). On misinterpreting thephylogenetic correction'. *Journal of Ecology*, *83*(3), 531–534.

Westoby, M., Yates, L., Holland, B., & Halliwell, B. (in press). Phylogenetically conservative trait correlation: Quantification and interpretation. *Journal of Ecology*.

Wiens, J. J., Ackerly, D. D., Allen, A. P., Anacker, B. L., Buckley, L. B., Cornell, H. V., Damschen, E. I., Jonathan Davies, T., Grytnes, J.-A., Harrison, S. P., et al. (2010). Niche conservatism as an emerging principle in ecology and conservation biology. *Ecology Letters*, *13*(10), 1310–1324.

Figure captions

Conceptual diagram of λ. For each λ transformation (given at the top) the resulting phylogeny is shown below (with arrows to indicate branch lengths in millions of years), and the phylogenetic variance-covariance (V_{phy}) matrix below that, and finally some comments on the transformation value below. Throughout, species' names are indicated with letters ('a', 'b', and 'c'). A λ of 1 leaves the tree unchanged (marked in red), while a λ of 0 transforms the phylogeny into a so-called 'star phylogeny' where essentially all phylogenetic information has been lost. The largest value of λ has been chosen to demonstrate the upper limit of λ in this phylogeny, where a further increase in λ would return off-diagonal elements ($\lambda \cdot \sigma 1, 2$ and $\lambda \cdot \sigma_{2,1}$) greater than one of the diagonal elements (σ_1^2), rendering V_{phy} improper. Conceptually, such a transformation reflects the impossibility of stretching the youngest node out beyond the present.
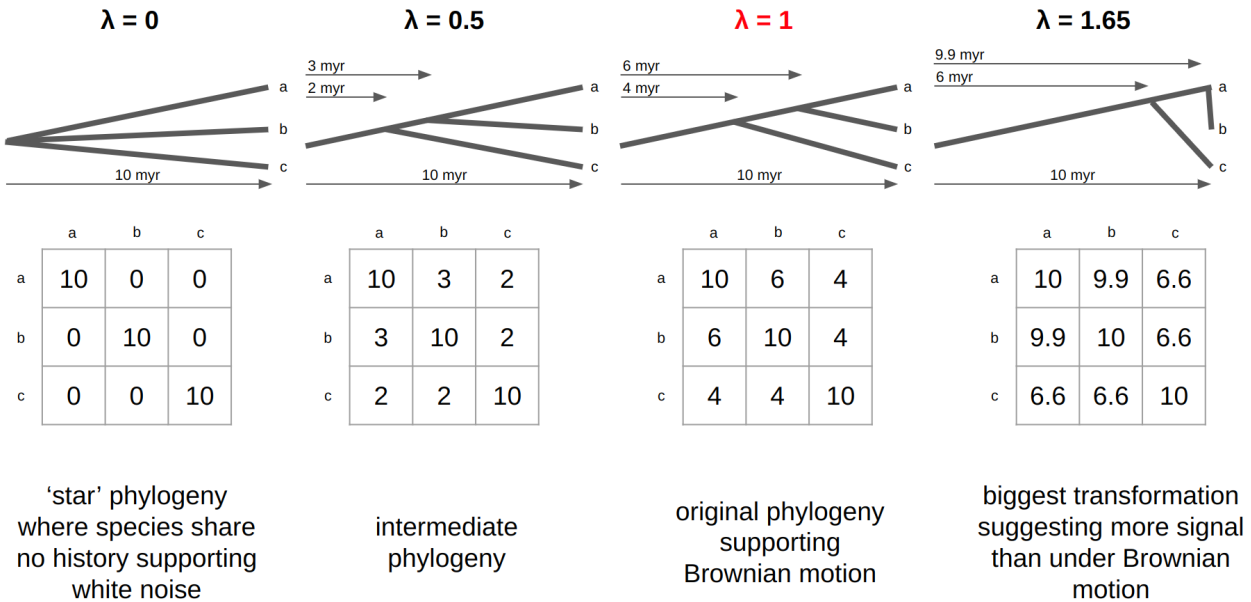
Figures

Figure 1: