

Phylogenetic Models

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Back to the Rhinograds: Phylogenetic Structural Equation Models with `because`

One of the core features of `because` is the ability to fit phylogenetic structural equation models (PSEMs), allowing researchers to account for shared evolutionary history among species when analysing trait relationships.

Once again we will use the Rhinogradentia dataset and tree previously analysed in Gonzalez-Voyer and von Hardenberg, (2014) and in von Hardenberg and Gonzalez-Voyer (2025). Let's start by loading the necessary packages and data:

```
library(because)
library(ape)

data(rhino.dat)
data(rhino.tree)
```

While in previous implementations it was necessary to compute the variance-covariance matrix from the tree and pass it to JAGS, `because` handles this internally. You only need to provide the phylogenetic tree (class `phylo`) via the `structure` argument. Also, `because` automatically matches the species names in the data and tree: you only need to ensure that the species names in the data frame column specified by `species` match the tip labels in the tree and provide the name of the species column to the `because()` function through the `id_col` argument. Also, you do not need to rescale the total tree length to 1 (needed for a correct estimation of Pagel's lambda parameter), as `because` will handle this internally.

So, let's specify the structural equations of the best model (`sem8`) as fitted by von Hardenberg and Gonzalez-Voyer (2025):

```
sem8_eq <- list(
  LS ~ BM,
  NL ~ BM + RS,
  DD ~ NL
)
```

Now we can fit the model with `because()` including the phylogenetic tree with the `structure` argument. Also, as this is a more complex model than in the previous examples, to speed up the model fitting we will run 3 chains in parallel using the `parallel = TRUE` and `n.cores = 3` arguments. Also we will request the WAIC information criterion to be computed by setting `WAIC = TRUE`:

```
fit_sem8 <- because(
  equations = sem8_eq,
  data = rhino.dat,
  structure = rhino.tree,
  id_col = "SP",
  WAIC = TRUE,
  parallel = TRUE,
  n.cores = 3
```

```
)
summary(fit_sem8)

summary(fit_sem8)
      Mean      SD Naive SE Time-series SE   2.5%    50% 97.5%
alphaDD      0.581  0.276    0.005        0.007  0.036  0.582 1.146
alphaLS      0.344  0.416    0.008        0.016 -0.490  0.346 1.138
alphaNL     -0.055  0.339    0.006        0.015 -0.731 -0.054 0.601
beta_DD_NL    0.536  0.074    0.001        0.001  0.390  0.538 0.682
beta_LS_BM    0.472  0.085    0.002        0.002  0.309  0.470 0.641
beta_NL_BM    0.470  0.068    0.001        0.001  0.336  0.471 0.604
beta_NL_RS    0.597  0.068    0.001        0.001  0.461  0.596 0.728
lambdaDD     0.462  0.130    0.002        0.003  0.218  0.462 0.717
lambdaLS     0.696  0.107    0.002        0.003  0.459  0.709 0.862
lambdaNL     0.719  0.086    0.002        0.002  0.533  0.727 0.863
sigma_DD_phylo 0.803  0.174    0.003        0.003  0.503  0.790 1.178
sigma_DD_res   0.856  0.088    0.002        0.002  0.694  0.852 1.041
sigma_LS_phylo 1.253  0.204    0.004        0.005  0.865  1.246 1.675
sigma_LS_res   0.804  0.104    0.002        0.002  0.615  0.802 1.013
sigma_NL_phylo 1.026  0.145    0.003        0.004  0.766  1.013 1.338
sigma_NL_res   0.626  0.075    0.001        0.002  0.490  0.622 0.783
      Rhat n.eff
alphaDD      1.000  1408
alphaLS      1.003  639
alphaNL      1.000  553
beta_DD_NL    1.000  3088
beta_LS_BM    1.001  2178
beta_NL_BM    1.000  2255
beta_NL_RS    1.001  2801
lambdaDD     1.002  2136
lambdaLS     1.000  1595
lambdaNL     1.001  1788
sigma_DD_phylo 1.002  2741
sigma_DD_res   1.000  2712
sigma_LS_phylo 1.000  1612
sigma_LS_res   1.001  2103
sigma_NL_phylo 1.001  1600
sigma_NL_res   1.001  2427

DIC:
Mean deviance: 670
penalty 133.7
Penalized deviance: 803.6

WAIC:
WAIC with Standard Errors
-----
N = 300 observations, 3000 MCMC samples

      Estimate      SE
elpd_waic   -395.1  9.9
p_waic       93.7  5.1
waic         790.2 19.8
```

The output shows that the posterior parameters are consistent with those we obtained coding the model directly in JAGS (von Hardenberg and Gonzalez-Voyer, 2025; the code is available in the supplementary materials of the paper).

The random effects formulation of because

If you are familiar with the output obtained from that model, you may however have noticed that besides Pagel's λ parameters for each response variable, with `because()` we also get estimates of the standard deviations of the phylogenetic and residual components (`sigma_[RESP]_phylo` and `sigma_[RESP]_res`, respectively). These are estimated because `because` uses an optimised random effect formulation to improve MCMC and significantly reduce runtime. While standard phylogenetic models must invert the covariance matrix at every iteration (as λ changes), the random effect approach is mathematically equivalent but computationally more efficient. `because` decomposes the response into three additive components:

$$y_i = \mu_i + u_i + \epsilon_i$$

where:

- μ_i is the fixed effect (structural equation mean)
- u_i is the phylogenetic random effect: $\mathbf{u} \sim \mathcal{N}(\mathbf{0}, \sigma_u^2 \mathbf{V})$
- ϵ_i is the residual error: $\epsilon \sim \mathcal{N}(\mathbf{0}, \sigma_e^2 \mathbf{I})$

This allows us to pre-compute the inverse phylogenetic variance-covariance matrix (\mathbf{V}^{-1}) only once and pass it to JAGS as fixed data. JAGS simply scales this fixed precision matrix by $1/\sigma$, avoiding costly repeated inversions.

Consequently, λ is derived from the posterior variance components as:

$$\lambda = \frac{\sigma_{phylo}^2}{\sigma_{phylo}^2 + \sigma_{res}^2}$$

This is the approach also used in other packages such as `MCMCglmm` (Hadfield, 2010) and `brms` (Bürkner, 2017).

Improved WAIC calculation

In `because` we also improved the WAIC calculation. The WAIC is now computed directly from the pointwise log-likelihoods monitored during model fitting, rather than approximating it from the deviance as done previously. This approach, besides providing more accurate estimates of the WAIC than the deviance-based approximation provided by JAGS, also allows us to compute the standard errors for WAIC (following the method suggested by Vehtari et al. 2017) allowing for more reliable model comparisons.

Testing conditional independencies with d-separation

Let's now test the conditional independencies implied by the model (We will set `WAIC = FALSE` here to speed up the computation, as we do not need to compare models):

```
test_sem8_dsep <- because(
  equations = sem8_eq,
  data = rhino.dat,
  structure = rhino.tree,
  id_col = "SP",
  dsep = TRUE,
  WAIC = FALSE,
  parallel = TRUE,
  n.cores = 3
)
```

d-separation Tests

```
Test: RS _||_ BM | {}
Parameter Estimate LowerCI UpperCI Indep      P   Rhat n.eff
beta_RS_BM    -0.029  -0.238   0.177   Yes 0.78 1.002  2177

Test: RS _||_ DD | {NL}
Parameter Estimate LowerCI UpperCI Indep      P   Rhat n.eff
beta_RS_DD    -0.117  -0.33    0.107   Yes 0.301 1       2563

Test: RS _||_ LS | {BM}
Parameter Estimate LowerCI UpperCI Indep      P   Rhat n.eff
beta_RS_LS    -0.019  -0.248   0.22    Yes 0.873 1       2423

Test: BM _||_ DD | {NL}
Parameter Estimate LowerCI UpperCI Indep      P   Rhat n.eff
beta_BM_DD    0.117  -0.111   0.342   Yes 0.322 1       1824

Test: NL _||_ LS | {RS,BM}
Parameter Estimate LowerCI UpperCI Indep      P   Rhat n.eff
beta_NL_LS    0.013  -0.151   0.177   Yes 0.86   1       2134

Test: DD _||_ LS | {NL,BM}
Parameter Estimate LowerCI UpperCI Indep      P   Rhat n.eff
beta_DD_LS    -0.063  -0.245   0.114   Yes 0.495 1.002  2693
```

Legend:

Indep: 'Yes' = Conditionally Independent, 'No' = Dependent (based on 95% CI)
P: Bayesian probability that the posterior distribution overlaps with zero

As expected, all conditional independencies are supported, indicating that the hypothesised causal structure is consistent with the data.

Accounting for variability in traits in PhyBaSE models

In von Hardenberg and Gonzalez-Voyer (2025), we showed how PhyBaSE models can be specified to account for measurement error or intraspecific variability in the traits. These models can also be fitted with `because()`. In the case of repeated measures per species, it is sufficient to provide the data frame with all measurements (i.e. multiple rows per species) and specify the `id_col` argument to indicate the species identifier column. `because()` will automatically format the data to create a response matrix with species in rows and replicates in columns, padding with NAs as necessary. As an example, we will use the same simulated data as in von Hardenberg and Gonzalez-Voyer (2025):

##References Vehtari, A., Gelman, A., & Gabry, J. (2017). Practical Bayesian model evaluation using leave-one-out cross-validation and WAIC. *Statistics and Computing*, 27(5), 1413-1432.