Appendix A: Comparison with other packages

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```
library(phylosem)
#> Loading required package: TMB
#> Warning: package 'TMB' was built under R version 4.3.1
```

```
message("Must install ggplot2, phylopath, phylolm, ape")
```

`phylosem` is an R package for fitting phylogenetic structural equation models (PSEMs). The package generalizes features in existing R packages:

- `sem` for structural equation models (SEMs);
- `phylosem` for comparison among alternative path models;
- `phylolm` for fitting large linear models that arise as when specifying a SEM with one endogenous variable and multiple exogenous and independent variables;
- `Rphylopars` for interpolating missing values when specifying a SEM with an unstructured (full rank) covariance among variables;

In model configurations that can be fitted by both `phylosem` and these other packages, we have confirmed that results are nearly identical or otherwise identified reasons that results differ.

`phylosem` involves a simple user-interface that specifies the SEM using notation from package `sem` and the phylogenetic tree using package `ape`. It allows uers to specify common models for the covariance including:

- Brownian motion (BM);
- Ornstein-Uhlenbeck (OU);
- Pagel's lambda;
- Pagel's kappa;

Output can be coerced to standard formats so that `phylosem` can use plotting and summary functions form other packages. Available output formats include:

- `sem`, for plotting the estimated SEM and summarizing direct and indirect effects;
- `phylopath`, for plotting and model comparison;
- `phylo4d` in R-package `phylobase` for plotting estimated traits;

Below, we specifically highlight the syntax, runtime, and output resulting from `phylosem` and other packages.

Comparison with phylolm

We first compare syntax and run-times using simulated data against `phylolm`. This confirms that runtimes from `phylosem` are within an order of magnitude and that results are nearly identical for BM, OU, delta, and kappa models.

```r
# Settings
Ntree = 100
sd_x = 0.3
sd_y = 0.3
b0_x = 1
b0_y = 0
b_xy = 1

# Simulate tree
set.seed(1)
tree = ape::rtree(n=Ntree)

# Simulate data
x = b0_x + sd_x * phylolm::rTrait(n = 1, phy=tree)
ybar = b0_y + b_xy*x
y_normal = ybar + sd_y * phylolm::rTrait(n = 1, phy=tree)

# Construct, re-order, and reduce data
Data = data.frame(x=x,y=y_normal)[]

# Compare using BM model
start_time = Sys.time()
plm_bm = phylolm::phylolm(y ~ 1 + x, data=Data, phy=tree, model="BM" )
Sys.time() - start_time
#> Time difference of 0.004724979 secs
knitr::kable(summary(plm_bm)$coefficients, digits=3)
```

	Estimate	StdErr	t.value	p.value
(Intercept)	-0.371	0.214	-1.734	0.086
x	1.117	0.101	11.053	0.000

```r
start_time = Sys.time()
psem_bm = phylosem( sem = "x -> y, p",
          data = Data,
          tree = tree,
          quiet = TRUE )
#> 1 regions found.
#> Using 1 threads
#> 1 regions found.
#> Using 1 threads
Sys.time() - start_time
#> Time difference of 0.183883 secs
knitr::kable(summary(psem_bm)$coefficients, digits=3)
```

Path	VarName	Estimate	StdErr	t.value	p.value
NA	Intercept_x	1.087	0.183	5.945	0.000
NA	Intercept_y	-0.371	0.213	1.743	0.081
x -> y	p	1.117	0.101	11.109	0.000
x <-> x	V[x]	0.315	0.022	14.072	0.000

Path	VarName	Estimate	StdErr	t.value	p.value
y <-> y	V[y]	0.315	0.022	14.072	0.000

```
# Compare using OU
start_time = Sys.time()
plm_ou = phylolm::phylolm(y ~ 1 + x, data=Data, phy=tree, model="OUrandomRoot" )
Sys.time() - start_time
#> Time difference of 0.1650479 secs

start_time = Sys.time()
psem_ou = phylosem( sem = "x -> y, p",
          data = Data,
          tree = tree,
          estimate_ou = TRUE,
          quiet = TRUE )
Sys.time() - start_time
#> Time difference of 0.1485529 secs

knitr::kable(summary(psem_ou)$coefficients, digits=3)
```

Path	VarName	Estimate	StdErr	t.value	p.value
NA	Intercept_x	1.028	0.208	4.946	0.000
NA	Intercept_y	-0.274	0.235	1.165	0.244
x -> y	p	1.099	0.101	10.887	0.000
x <-> x	V[x]	0.332	0.026	12.712	0.000
y <-> y	V[y]	0.332	0.026	12.860	0.000

```
knitr::kable(summary(plm_ou)$coefficients, digits=3)
```

	Estimate	StdErr	t.value	p.value
(Intercept)	-0.781	0.389	-2.006	0.048
x	1.095	0.101	10.850	0.000

```
knitr::kable(c( "phylolm_alpha"=plm_ou$optpar,
                "phylosem_alpha"=exp(psem_ou$parhat$lnalpha) ), digits=3)
```

	x
phylolm_alpha	0.120
phylosem_alpha	0.105

```
# Compare using Pagel's lambda
start_time = Sys.time()
plm_lambda = phylolm::phylolm(y ~ 1 + x, data=Data, phy=tree, model="lambda" )
Sys.time() - start_time
#> Time difference of 0.01492906 secs
```

```
start_time = Sys.time()
psem_lambda = phylosem( sem = "x -> y, p",
          data = Data,
          tree = tree,
          estimate_lambda = TRUE,
          quiet = TRUE )
Sys.time() - start_time
#> Time difference of 0.1191969 secs

knitr::kable(summary(psem_lambda)$coefficients, digits=3)
```

Path	VarName	Estimate	StdErr	t.value	p.value
NA	Intercept_x	1.092	0.162	6.740	0.000
NA	Intercept_y	-0.346	0.200	1.726	0.084
x -> y	p	1.092	0.103	10.559	0.000
x <-> x	V[x]	0.284	0.025	11.367	0.000
y <-> y	V[y]	0.290	0.024	11.897	0.000

```
knitr::kable(summary(plm_lambda)$coefficients, digits=3)
```

	Estimate	StdErr	t.value	p.value
(Intercept)	-0.356	0.207	-1.718	0.089
x	1.102	0.103	10.744	0.000

```
knitr::kable(c( "phylolm_lambda"=plm_lambda$optpar,
                "phylosem_lambda"=plogis(psem_lambda$parhat$logitlambda) ), digits=3)
```

	x
phylolm_lambda	0.980
phylosem_lambda	0.957

```
# Compare using Pagel's kappa
start_time = Sys.time()
plm_kappa = phylolm::phylolm(y ~ 1 + x, data=Data, phy=tree, model="kappa", lower.bound = 0, upper.bound
Sys.time() - start_time
#> Time difference of 0.005271912 secs

start_time = Sys.time()
psem_kappa = phylosem( sem = "x -> y, p",
          data = Data,
          tree = tree,
          estimate_kappa = TRUE,
          quiet = TRUE )
Sys.time() - start_time
#> Time difference of 0.1185069 secs

knitr::kable(summary(psem_kappa)$coefficients, digits=3)
```

Path	VarName	Estimate	StdErr	t.value	p.value
NA	Intercept_x	1.078	0.186	5.783	0.000
NA	Intercept_y	-0.368	0.216	1.705	0.088
x -> y	p	1.113	0.101	11.025	0.000
x <-> x	V[x]	0.299	0.029	10.183	0.000
y <-> y	V[y]	0.300	0.029	10.343	0.000

```r
knitr::kable(summary(plm_kappa)$coefficients, digits=3)
```

	Estimate	StdErr	t.value	p.value
(Intercept)	-0.370	0.216	-1.716	0.089
x	1.115	0.101	11.015	0.000

```r
knitr::kable(c( "phylolm_kappa"=plm_kappa$optpar,
                "phylosem_kappa"=exp(psem_kappa$parhat$lnkappa) ), digits=3)
```

	x
phylolm_kappa	0.930
phylosem_kappa	0.857

Generalized linear models

We also compare results among software for fitting phylogenetic generalized linear models (PGLM).

Poisson-distributed response

First, we specifically explore a Poisson-distributed PGLM, comparing `phylosem` against `phylolm::phyloglm` (which uses Generalized Estimating Equations) and `phyr::pglmm_compare` (which uses maximum likelihood).

```r
# Settings
Ntree = 100
sd_x = 0.3
sd_y = 0.3
b0_x = 1
b0_y = 0
b_xy = 1

# Simulate tree
set.seed(1)
tree = ape::rtree(n=Ntree)

# Simulate data
x = b0_x + sd_x * phylolm::rTrait(n = 1, phy=tree)
ybar = b0_y + b_xy*x
y_normal = ybar + sd_y * phylolm::rTrait(n = 1, phy=tree)
y_pois = rpois( n=Ntree, lambda=exp(y_normal) )
```

```r
# Construct, re-order, and reduce data
Data = data.frame(x=x,y=y_pois)

# Compare using phylolm::phyloglm
pglm = phylolm::phyloglm(y ~ 1 + x, data=Data, phy=tree, method="poisson_GEE" )
knitr::kable(summary(pglm)$coefficients, digits=3)
```

	Estimate	StdErr	z.value	p.value
(Intercept)	-1.098	0.633	-1.736	0.083
x	1.314	0.247	5.320	0.000

```r
#
pglmm = phyr::pglmm_compare(
  y ~ 1 + x,
  family = "poisson",
  data = Data,
  phy = tree )
knitr::kable(summary(pglmm), digits=3)
#> Generalized linear mixed model for poisson data fit by restricted maximum likelihood
#>
#> Call:y ~ 1 + x
#>
#> logLik    AIC    BIC
#> -173.4  354.7  360.6
#>
#> Phylogenetic random effects variance (s2):
#>    Variance Std.Dev
#> s2  0.05511  0.2348
#>
#> Fixed effects:
#>                Value Std.Error  Zscore    Pvalue
#> (Intercept) -0.57009   0.30469 -1.8710   0.06134 .
#> x            1.18137   0.19807  5.9645 2.454e-09 ***
#> ---
#> Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```r
#
pgsem = phylosem( sem = "x -> y, p",
          data = Data,
          family = c("fixed","poisson"),
          tree = tree,
          quiet = TRUE )
knitr::kable(summary(pgsem)$coefficients, digits=3)
```

Path	VarName	Estimate	StdErr	t.value	p.value
NA	Intercept_x	1.087	0.183	5.945	0.000
NA	Intercept_y	-0.581	0.305	1.904	0.057
x -> y	p	1.190	0.199	5.971	0.000

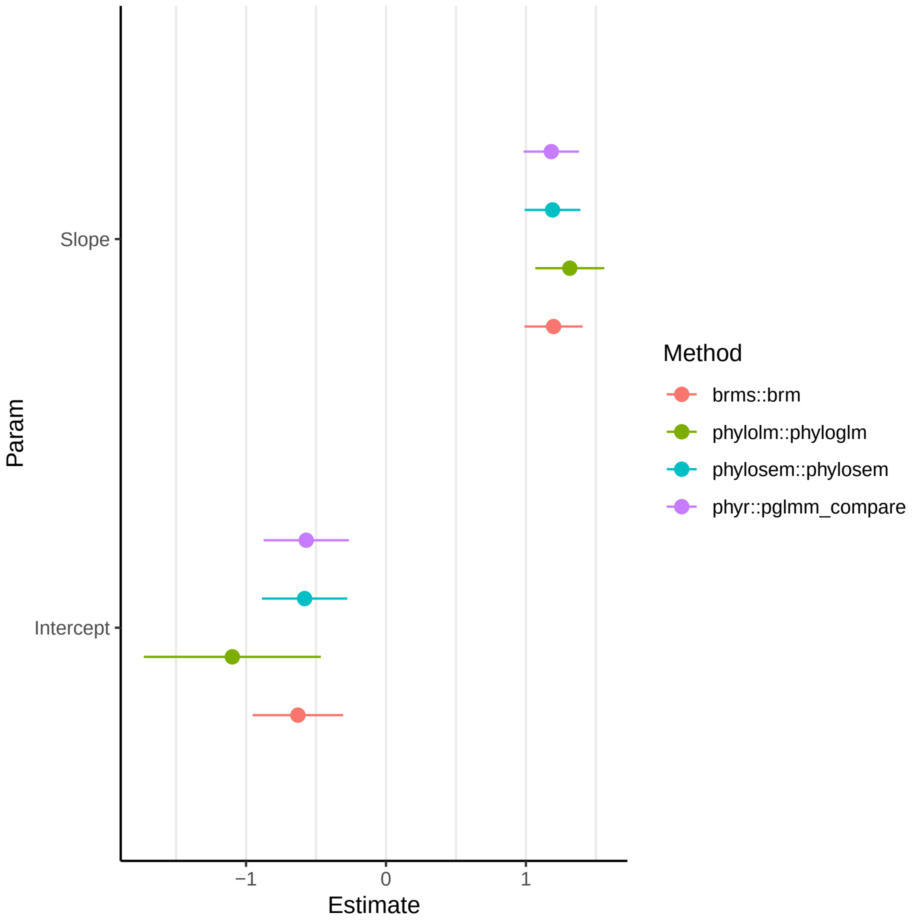
Path	VarName	Estimate	StdErr	t.value	p.value
x <-> x	V[x]	0.315	0.022	14.072	0.000
y <-> y	V[y]	0.232	0.054	4.310	0.000

We also compare results against `brms` (which fits a Bayesian hierarchical model), although we load results from compiled run of `brms` to avoid users having to install STAN to run vignettes for `phylosem`:

```r
# Comare using Bayesian implementation in brms
library(brms)
Amat <- ape::vcv.phylo(tree)
Data$tips <- rownames(Data)
mcmc <- brm(
  y ~ 1 + x + (1 | gr(tips, cov = A)),
  data = Data, data2 = list(A = Amat),
  family = 'poisson',
  cores = 4
)
knitr::kable(fixef(mcmc), digits = 3)

# Plot them together
library(ggplot2)
pdat <- rbind.data.frame(
  coef(summary(pglm))[, 1:2],
  data.frame(Estimate = pglmm$B, StdErr = pglmm$B.se),
  setNames(as.data.frame(fixef(mcmc))[1:2], c('Estimate', 'StdErr')),
  setNames(summary(pgsem)$coefficients[2:3, 3:4], c('Estimate', 'StdErr'))
)
pdat$Param <- rep(c('Intercept', 'Slope'), 4)
pdat$Method <- rep( c('phylolm::phyloglm', 'phyr::pglmm_compare',
                     'brms::brm', 'phylosem::phylosem'), each = 2)
figure = ggplot(pdat, aes(
  x = Estimate, xmin = Estimate - StdErr,
  xmax = Estimate + StdErr, y = Param, color = Method
)) +
  geom_pointrange(position = position_dodge(width = 0.6)) +
  theme_classic() +
  theme(panel.grid.major.x = element_line(), panel.grid.minor.x = element_line())
saveRDS( figure, file=file.path(R'(C:\Users\James.Thorson\Desktop\Git\phylosem\vignettes)',"brms.RDS")
```

```
#> Warning: package 'ggplot2' was built under R version 4.3.1
```



In this instance (and in others we have explored), results from `phylolm::phyloglm` are generally different while those from `phylosem`, `phyr::pglmm_compare`, and `brms` are close but not quite identical.

Binomial regression

We also compare results for a Bernoulli-distributed response using PGLM. We again compare `phylosem` against `phyr::pglmm_compare`, and do not explore threshold models which we expect to give different results due differences in assumptions about how latent variables affect measurements.

```
# Settings
Ntree = 100
sd_x = 0.3
sd_y = 0.3
b0_x = 1
b0_y = 0
b_xy = 1

# Simulate tree
set.seed(1)
tree = ape::rtree(n=Ntree)

# Simulate data
x = b0_x + sd_x * phylolm::rTrait(n = 1, phy=tree)
```

```r
ybar = b0_y + b_xy*x
y_normal = ybar + sd_y * phylolm::rTrait(n = 1, phy=tree)
y_binom = rbinom( n=Ntree, size=1, prob=plogis(y_normal) )

# Construct, re-order, and reduce data
Data = data.frame(x=x,y=y_binom)

#
pglmm = phyr::pglmm_compare(
  y ~ 1 + x,
  family = "binomial",
  data = Data,
  phy = tree )
knitr::kable(summary(pglmm), digits=3)
#> Generalized linear mixed model for binomial data fit by restricted maximum likelihood
#>
#> Call:y ~ 1 + x
#>
#> logLik    AIC    BIC
#> -63.74 135.47 141.32
#>
#> Phylogenetic random effects variance (s2):
#>    Variance Std.Dev
#> s2   0.1076   0.328
#>
#> Fixed effects:
#>               Value Std.Error Zscore Pvalue
#> (Intercept) 0.23179   0.60507 0.3831 0.7017
#> x           0.44548   0.45708 0.9746 0.3297
```

```r
#
pgsem = phylosem( sem = "x -> y, p",
          data = Data,
          family = c("fixed","binomial"),
          tree = tree,
          quiet = TRUE )
knitr::kable(summary(pgsem)$coefficients, digits=3)
```

Path	VarName	Estimate	StdErr	t.value	p.value
NA	Intercept_x	1.087	0.183	5.945	0.000
NA	Intercept_y	0.204	0.589	0.346	0.730
x -> y	p	0.458	0.468	0.977	0.328
x <-> x	V[x]	-0.315	0.022	14.072	0.000
y <-> y	V[y]	0.290	0.284	1.020	0.308

In this instance, `phylosem` and `phyr::pglmm_compare` give similar estimates and standard errors for the slope term.

Summary of PGLM results

Based on these two comparisons, we conclude that phylosem provides an interface for maximum-likelihood estimate of phylogenetic generalized linear models (PGLM), and extends this class to include mixed data (i.e., a combination of different measurement types), missing data, and non-recursive structural linkages. However, we also encourage further cross-testing of different software for fitting phylogenetic generalized linear models.

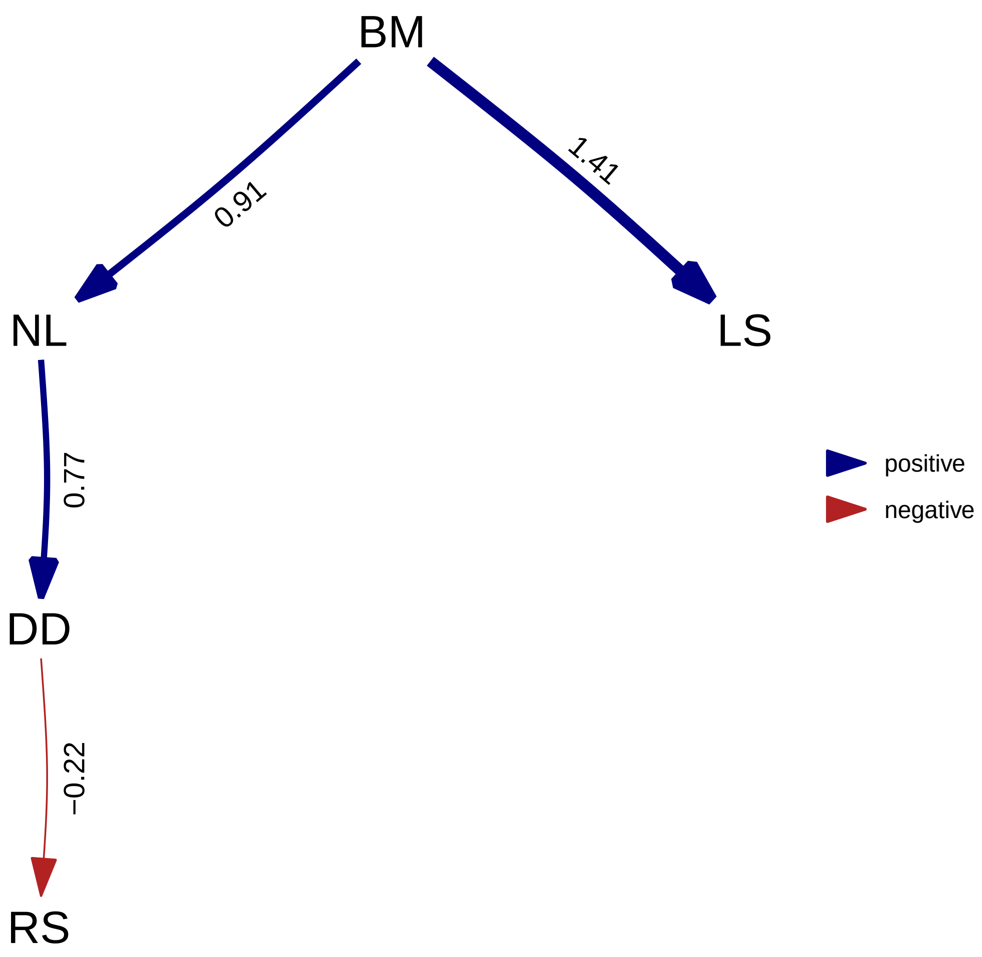
Compare with phylopath

We next compare with a single run of `phylopath`. This again confirms that runtimes are within an order of magnitude and results are identical for standardized or unstandardized coefficients.

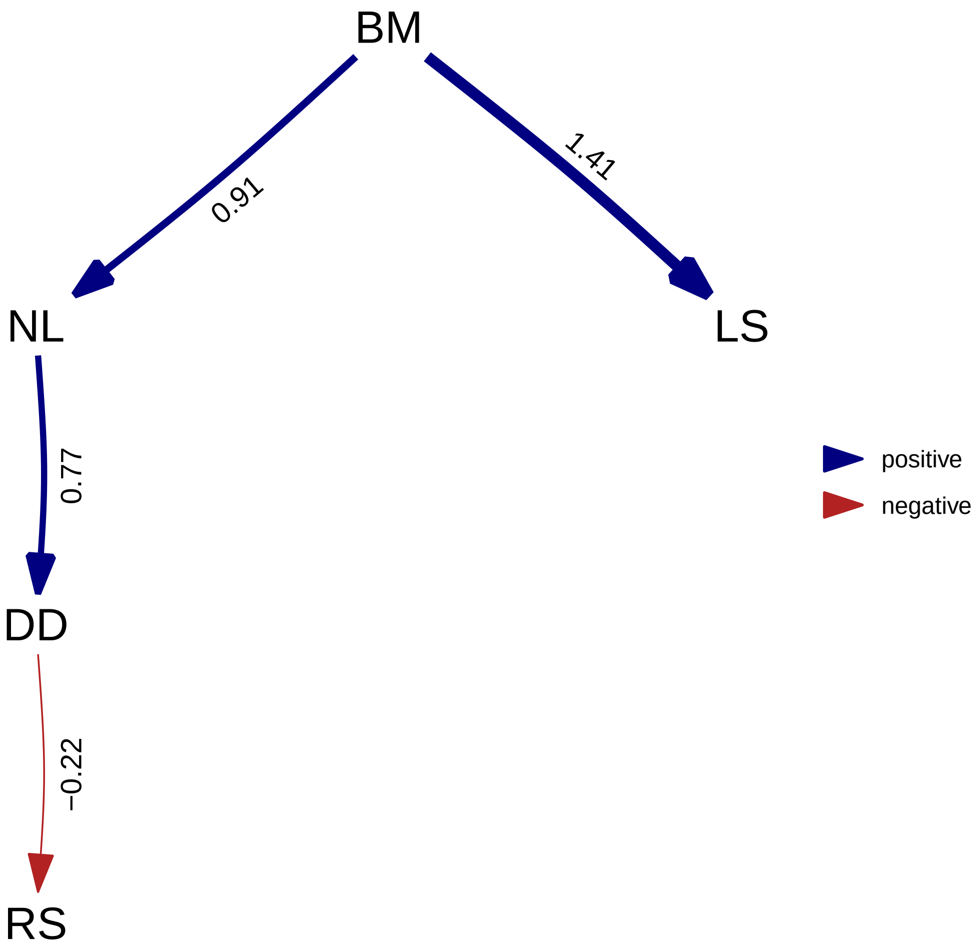
```
library(phylopath)
#> Warning: package 'phylopath' was built under R version 4.3.1
library(phylosem)

# make copy of data that's rescaled
rhino_scaled = rhino
  rhino_scaled[,c("BM","NL","LS","DD","RS")] = scale(rhino_scaled[,c("BM","NL","LS","DD","RS")])

# Fit and plot using phylopath
dag <- DAG(RS ~ DD, LS ~ BM, NL ~ BM, DD ~ NL)
start_time = Sys.time()
result <- est_DAG( DAG = dag,
                    data = rhino,
                    tree = rhino_tree,
                    model = "BM",
                    measurement_error = FALSE )
Sys.time() - start_time
#> Time difference of 0.007936001 secs
plot(result)
```



```
# Fit and plot using phylosem
model = "
  DD -> RS, p1
  BM -> LS, p2
  BM -> NL, p3
  NL -> DD, p4
"
start_time = Sys.time()
psem = phylosem( sem = model,
          data = rhino_scaled[,c("BM","NL","DD","RS","LS")],
          tree = rhino_tree,
          quiet = TRUE )
Sys.time() - start_time
#> Time difference of 0.1894739 secs
plot( as_fitted_DAG(psem) )
```



Comparison with sem

We next compare syntax and runtime against R-package `sem`. This confirms that runtimes are within an order of magnitude when specifying a star-phylogeny in `phylosem` to match the assumed structure in `sem`

```r
library(sem)
#> Warning: package 'sem' was built under R version 4.3.1
library(TreeTools)
#> Warning: package 'TreeTools' was built under R version 4.3.1
#> Warning: package 'ape' was built under R version 4.3.1

# Simulation parameters
n_obs = 50
# Intercepts
a1 = 1
a2 = 2
```

```
a3 = 3
a4 = 4
# Slopes
b12 = 0.3
b23 = 0
b34 = 0.3
# Standard deviations
s1 = 0.1
s2 = 0.2
s3 = 0.3
s4 = 0.4

# Simulate data
E1 = rnorm(n_obs, sd=s1)
E2 = rnorm(n_obs, sd=s2)
E3 = rnorm(n_obs, sd=s3)
E4 = rnorm(n_obs, sd=s4)
Y1 = a1 + E1
Y2 = a2 + b12*Y1 + E2
Y3 = a3 + b23*Y2 + E3
Y4 = a4 + b34*Y3 + E4
Data = data.frame(Y1=Y1, Y2=Y2, Y3=Y3, Y4=Y4)

# Specify path diagram (in this case, using correct structure)
equations = "
  Y2 = b12 * Y1
  Y4 = b34 * Y3
"
model <- specifyEquations(text=equations, exog.variances=TRUE, endog.variances=TRUE)

# Fit using package:sem
start_time = Sys.time()
Sem <- sem(model, data=Data)
Sys.time() - start_time
#> Time difference of 0.0115509 secs

# Specify star phylogeny
tree_null = TreeTools::StarTree(n_obs)
  tree_null$edge.length = rep(1,nrow(tree_null$edge))
  rownames(Data) = tree_null$tip.label

# Fit using phylosem
start_time = Sys.time()
psem = phylosem( data = Data,
          sem = equations,
          tree = tree_null,
          quiet = TRUE )
Sys.time() - start_time
#> Time difference of 0.03682089 secs
```

We then compare estimated values for standardized coefficients

	x
b12	0.326
b34	0.325

Path	Parameter	Estimate
Y1 -> Y2	b12	0.345
Y3 -> Y4	b34	0.343

and also compare values for unstandardized coefficients:

	x
b12	0.660
b34	0.390
V[Y1]	0.010
V[Y2]	0.038
V[Y3]	0.098
V[Y4]	0.126

Path	Parameter	Estimate
Y1 -> Y2	b12	0.660
Y3 -> Y4	b34	0.390
Y1 <-> Y1	V[Y1]	0.010
Y2 <-> Y2	V[Y2]	0.038
Y3 <-> Y3	V[Y3]	0.098
Y4 <-> Y4	V[Y4]	0.126

Comparison with Rphylopars

Finally, we compare syntax and runtime against R-package `Rphylopars`. This confirms that we can impute identical estimates using both packages, when specifying a full-rank covariance in `phylosem`

We note that `phylosem` also allows parsimonious representations of the trait covariance via the inputted SEM structure.

```
library(Rphylopars)

# Format data, within no values for species t1
Data = rhino[,c("BM","NL","DD","RS","LS")]
  rownames(Data) = tree$tip.label
Data['t1',] = NA

# fit using phylopars
start_time = Sys.time()
pars <- phylopars( trait_data = cbind(species=rownames(Data),Data),
                  tree = tree,
                  pheno_error = FALSE,
                  phylo_correlated = TRUE,
                  pheno_correlated = FALSE)
Sys.time() - start_time
#> Time difference of 0.08049917 secs

# Display estimates for missing values
knitr::kable(cbind( "Estimate"=pars$anc_recon["t1",], "Var"=pars$anc_var["t1",] ), digits=3)
```

	Estimate	Var
BM	1.266	1.941
NL	1.600	1.856
DD	2.301	1.708
RS	0.431	1.909
LS	1.083	1.347

```
# fit using phylosem
start_time = Sys.time()
psem = phylosem( data = Data,
                 tree = tree,
                 sem = "",
                 covs = "BM, NL, DD, RS, LS",
                 quiet = TRUE )
Sys.time() - start_time
#> Time difference of 0.302736 secs

# Display estimates for missing values
knitr::kable(cbind(
  "Estimate"=as.list(psem$opt$SD,"Estimate")$x_vj[ match("t1",tree$tip.label), ],
  "Var"=as.list(psem$opt$SD,"Std. Error")$x_vj[ match("t1",tree$tip.label), ]^2
), digits=3)
```

Estimate	Var
1.266	1.941
1.600	1.856
2.301	1.708
0.431	1.910
1.083	1.347