Appendix A: Comparison with other packages

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```r
library(phylosem)
```

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
```

```r
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 0.001960039 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 )
Sys.time() - start_time
#> Time difference of 0.07042909 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
y <-> y	V[y]	0.315	0.022	14.072	0.000

```r
# 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 0.007655859 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 0.1137979 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 0.01393509 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 0.08813381 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.boun
Sys.time() - start_time
#> Time difference of 0.004652023 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 0.1293001 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

Path	VarName	Estimate	StdErr	t.value	p.value
x <-> x	V[x]	0.299	0.029	10.183	0.000
y <-> y	V[y]	0.300	0.029	10.343	0.000

```
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

```
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).

```
# 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) )

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

```r
# Compare using 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
```

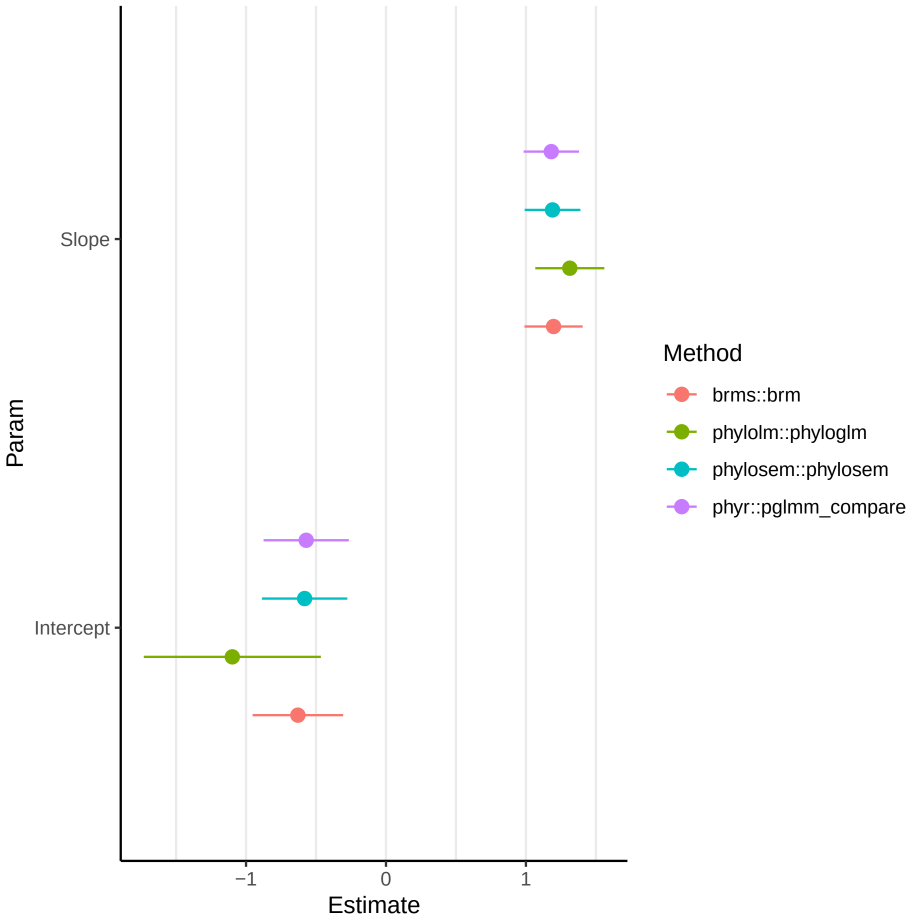
```r
#
pgsem = phylosem( sem = "x -> y, p",
          data = Data,
          family = c("fixed","poisson"),
          tree = tree,
          quiet = TRUE )
knitr::kable(summary(pgsem)$coefficients, digits=3)
```

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
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")
```



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)
```

```
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
```

```
#
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.

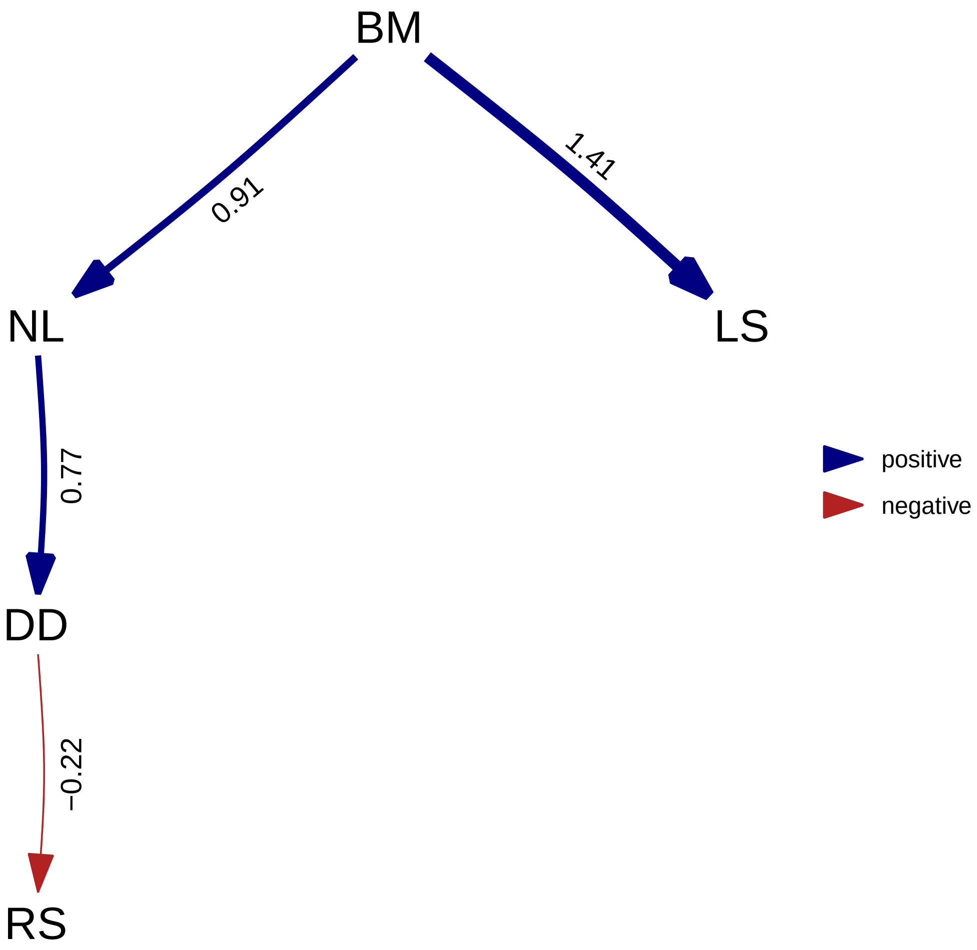
Compare with phylopath

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.

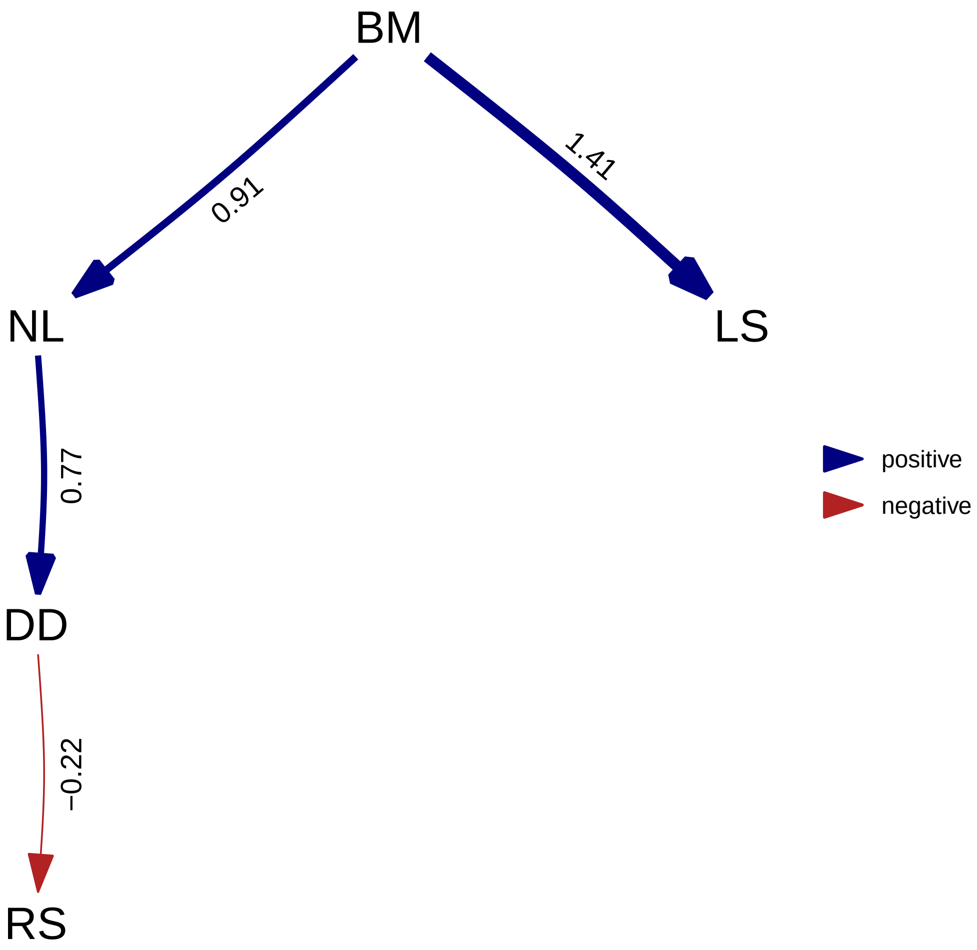
```
library(phylopath)
library(phylosem)

# 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 0.006084919 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 0.1849489 secs
plot( as(psem,"fitted_DAG") )
```



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`

```
library(sem)
library(TreeTools)

# Simulation parameters
n_obs = 50
# Intercepts
a1 = 1
a2 = 2
a3 = 3
a4 = 4
# Slopes
```

```r
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 0.004358053 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 0.03699112 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.

```r
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 0.07553792 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

```r
# 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 0.3031831 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