Appendix C: Demonstration of selected features

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```
library(phylosem)
```

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

phylosem is an R package for fitting phylogenetic structural equation models (PSEMs). We here highlight a few features in particular.

Estimability for multiple covariance transformations

By default, phylosem takes as input a phylogenetic tree and constructs a covariance under a Brownian motion evolutionary model. However, it also allows any combination of the following transformations:

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

This then results in eight possible covariance models formed from including or excluding each transformation. We first show that these transformations are all simultaneously estimable for a reference data set.

```
# Compare using Pagel's kappa
library(phylopath)

# Run phylosem
model = "
  DD -> RS, p1
  BM -> LS, p2
  BM -> NL, p3
  NL -> DD, p4
"
psem = phylosem( sem = model,
          data = rhino[,c("BM","NL","DD","RS","LS")],
          estimate_ou = TRUE,
          estimate_lambda = TRUE,
          estimate_kappa = TRUE,
          tree = rhino_tree,
          getJointPrecision = TRUE,
          quiet = TRUE )

#
V = psem$opt$SD$cov.fixed
Rsub = cov2cor(V)[c('lnalpha','logitlambda','lnkappa'),c('lnalpha','logitlambda','lnkappa')]
```

```r
knitr::kable(c("minimum_eigenvalue"=min(eigen(psem$opt$SD$jointPrecision)$values),
             "maximum_eigenvalue"=max(eigen(psem$opt$SD$jointPrecision)$values)), digits=3)
```

	x
minimum_eigenvalue	0.035
maximum_eigenvalue	43439.097

```r
knitr::kable(Rsub, digits=3)
```

	lnalpha	logitlambda	lnkappa
lnalpha	1.000	0.741	0.422
logitlambda	0.741	1.000	0.183
lnkappa	0.422	0.183	1.000

We see that the minimum eigenvalue for the precision matrix (which corresponds to the maximum eigenvalue of the covariance matrix) is greater than zero, such that the precision is invertible and the Hessian matrix is full rank. From this we can see that all parameters are estimable when applying all three transformations. We also see that transformation parameters are not perfectly correlated, although the logit-lambda and ln-alpha parameters have a correlation of approximately 0.75.

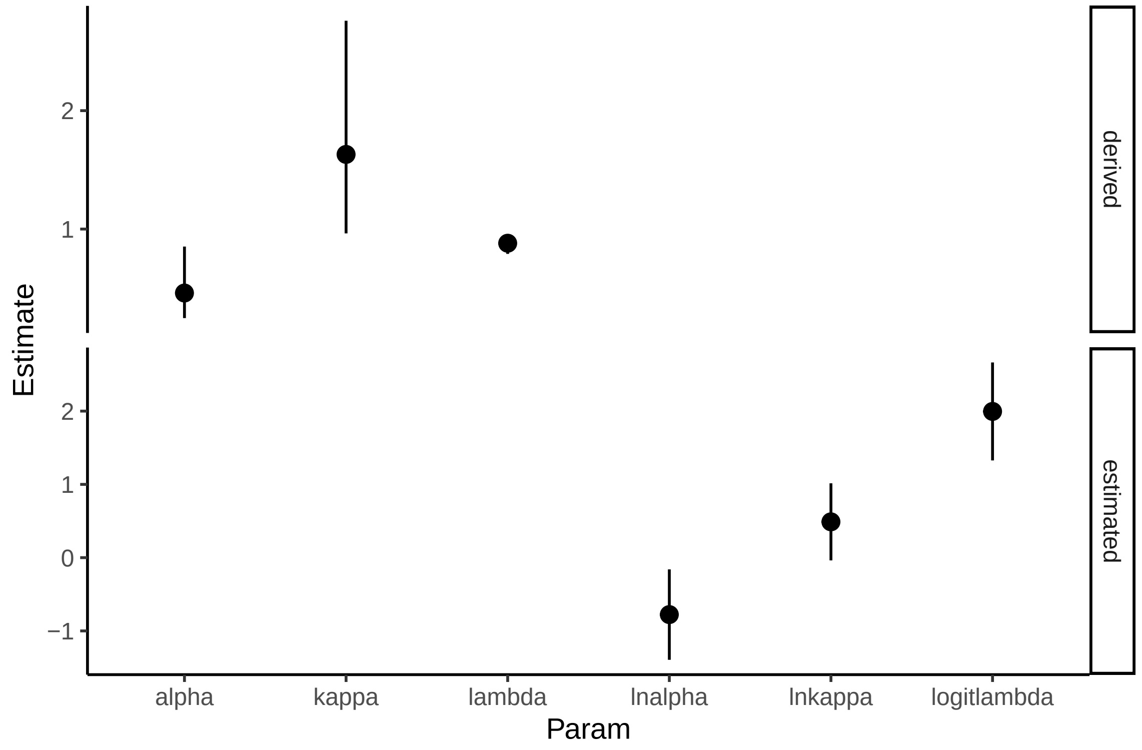
We can also extract the standard errors, calculated as the square-root of the diagonal elements of the covariance matrix. We extract the estimated values for `lnalpha`, `logitlambda`, and `lnkappa` and plot plot the 95% confidence interval as their estimates plus or minus 1.96 times their standard errors. These values are all unbounded by construction. However, we also convert these estimates, lower, and upper confidence-interval bounds to the conventional parameters `alpha`, `lambda`, and `kappa`, and plot those as well. These derived quantities are bounded as expected for Ornstein-Uhlenbeck and Pagel parameters:

```r
library(ggplot2)
# Compile estimates and SEs
pdat = data.frame( "Estimate" = psem$opt$SD$par.fixed[c('lnalpha','logitlambda','lnkappa')],
              "StdErr" = sqrt(diag(V)[c('lnalpha','logitlambda','lnkappa')]) )
pdat = cbind( pdat, "Param" = rownames(pdat))

#
pdat$lower = pdat$Estimate - 1.96*pdat$StdErr
pdat$upper = pdat$Estimate + 1.96*pdat$StdErr
pdat$type = "estimated"

# Transform from log / logit-space to natural space
pdat2 = pdat
pdat2$Param = c("alpha", "lambda", "kappa")
pdat2['lnalpha',c("Estimate","lower","upper")] = exp(pdat2['lnalpha',c("Estimate","lower","upper")])
pdat2['lnkappa',c("Estimate","lower","upper")] = exp(pdat2['lnkappa',c("Estimate","lower","upper")])
pdat2['logitlambda',c("Estimate","lower","upper")] = plogis(as.numeric(pdat2['logitlambda',c("Estimate"
pdat2$type = "derived"

# Plot
ggplot( rbind(pdat,pdat2), aes( x=Param, y = Estimate, ymin = lower, ymax = upper)) +
  geom_pointrange(position = position_dodge(width = 0.6)) +
  theme_classic() +
  facet_grid( rows=vars(type), scales="free" )
```



These confidence intervals suggest that parameter lnkappa overlaps with 0.0, suggesting that Pagel's kappa overlaps with 1.0 and could be instead turned off and thereby fixed at that default value.

Scaling of runtime with increased tree size

The package `phylolm` is expected to have a "linear runtime", i.e., a proportional increase in runtime with increasing tree size. We therefore compare runtime for `phylosem` and `phylolm` using a simulated tree across three orders of magnitude (10, 100, 1000, or 10000 tips).

```
# Settings
Ntree_config = c( 1e1, 1e2, 1e3, 1e4 )
Nreplicates = 5
sd_x = 0.3
sd_y = 0.3
b0_x = 1
b0_y = 0
b_xy = 1

# Simulate tree
set.seed(1)
Time_rcz = array(NA, dim=c(Nreplicates,length(Ntree_config),2), dimnames=list(NULL,"tree_size"=Ntree_co

for( rI in seq_len(Nreplicates) ){
for( cI in seq_along(Ntree_config) ){
```

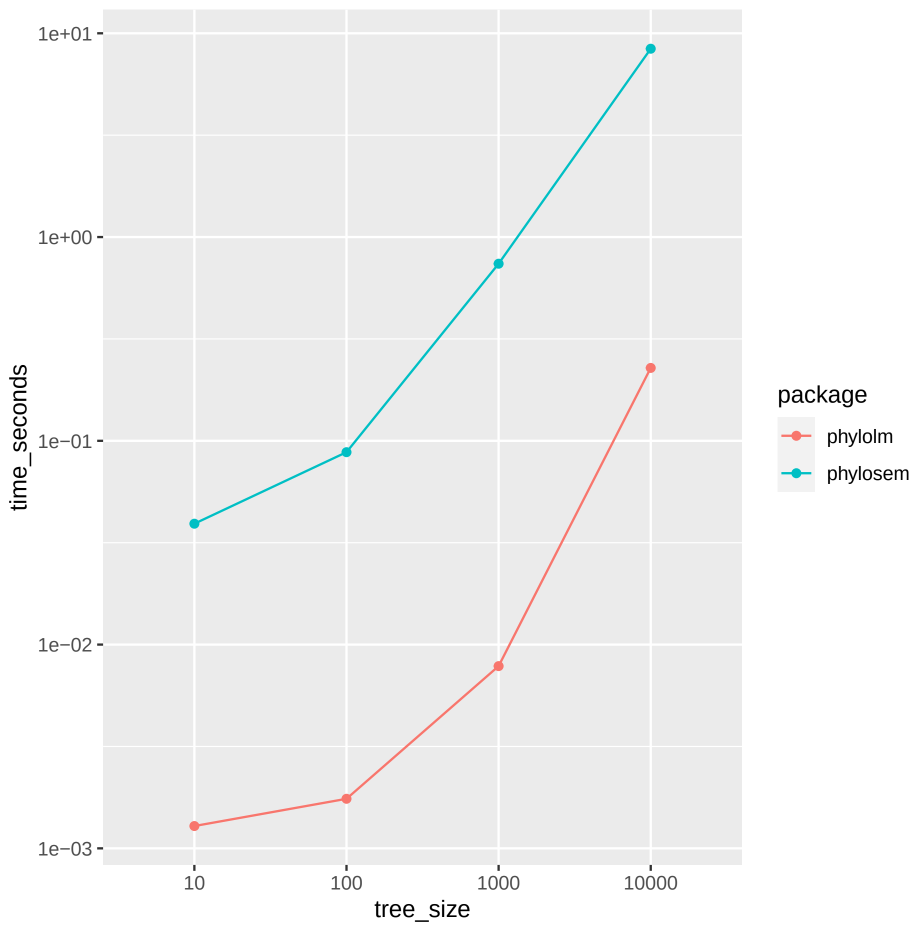
```r
  # Simulate data
  tree = ape::rtree(n=Ntree_config[cI])
  x = b0_x + sd_x * phylolm::rTrait(n = 1, phy=tree)
  ybar = b0_y + b_xy*x
  y_normal = ybar + sd_y * phylolm::rTrait(n = 1, phy=tree)
  Data = data.frame(x=x, y=y_normal)[]

  # Run phylolm
  start_time = Sys.time()
  plm_bm = phylolm::phylolm(y ~ 1 + x, data=Data, phy=tree, model="BM" )
  Time_rcz[rI,cI,"phylolm"] = Sys.time() - start_time

  # Run phylosem
  start_time = Sys.time()
  psem_bm = phylosem( sem = "x -> y, p",
            data = Data,
            tree = tree,
            quiet = TRUE,
            newtonsteps = 0,
            getsd = FALSE )
  Time_rcz[rI,cI,"phylosem"] = Sys.time() - start_time
}}

# Format
df = apply( Time_rcz, MARGIN=2:3, FUN=mean )
df = cbind( expand.grid(dimnames(df)), "time_seconds"=as.vector(df) )

# Plot
library(ggplot2)
ggplot(data=df, aes(x=tree_size, y=time_seconds, group=package, color=package)) +
  geom_line() +
  geom_point() + scale_y_log10()
```



Results show that both packages have approximately linear runtime, but that `phylolm` is approximately 10-100 times faster for any given tree size.