

Supplemental Material for 'Niche estimation above and below the species level'

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R code for comparing splitting, lumping, partial pooling, and phylogenetically-informed ecological niche models on a simulated dataset (*Box 3*)

This source code is archived in Zenodo (Rodríguez-Sánchez 2018) and can also be found at <https://github.com/Pakillo/phyloENM-TREE>.

Simulate taxa niches and phylogeny

Here we simulate (following Pearse *et al.* 2016) a group of phylogenetically related taxa with different sensitivities to temperature, so that closely related taxa will have more similar niches.

```
nspp <- 6
nsite <- 30

# simulate a phylogenetic tree
library(ape)
set.seed(6)
```

```

phy <- rtree(n = nspp)
phy <- compute.brlen(phy, method = "Grafen", power = 0.5)
#plot(phy)

# standardize the phylogenetic covariance matrix to have determinant 1
Vphy <- vcv(phy)
Vphy.std <- Vphy/(det(Vphy)^(1/nspp))

# Perform a Cholesky decomposition of Vphy
iD <- t(chol(Vphy.std))

# Generate environmental site variable
env <- seq(0, 20, length.out = nsite)

## Set up species-specific regression coefficients as random effects

set.seed(79)

intercept <- iD %*% runif(nspp, -1, 2)
slope <- iD %*% runif(nspp, -0.4, 0.1)

intercept <- intercept[gtools::mixedorder(rownames(intercept)), ]
slope <- slope[gtools::mixedorder(rownames(slope)), ]

#intercept
#slope

## Calculate suitabilities for each taxa and site

```

```

suitab <- rep(intercept, each = nsite)
suitab <- suitab + rep(slope, each = nsite) * rep(env, nspp)
suitab.error <- suitab + rnorm(nspp * nsite, mean = 0, sd = 1) #add some random 'error'
suitab.invlogit <- arm::invlogit(suitab)
suitab.error.invlogit <- arm::invlogit(suitab.error)

set.seed(114)

pres <- rbinom(length(suitab.error), size = 1, prob = suitab.error.invlogit) # pres-abs

dat <- data.frame(taxa = paste("t", sort(rep(1:nspp, nsite))), sep = ""),
                  site = rep(1:nsite, nspp),
                  env = rep(env, nspp),
                  suitab.invlogit = suitab.invlogit,
                  presabs = pres)

```

Plot simulated niches

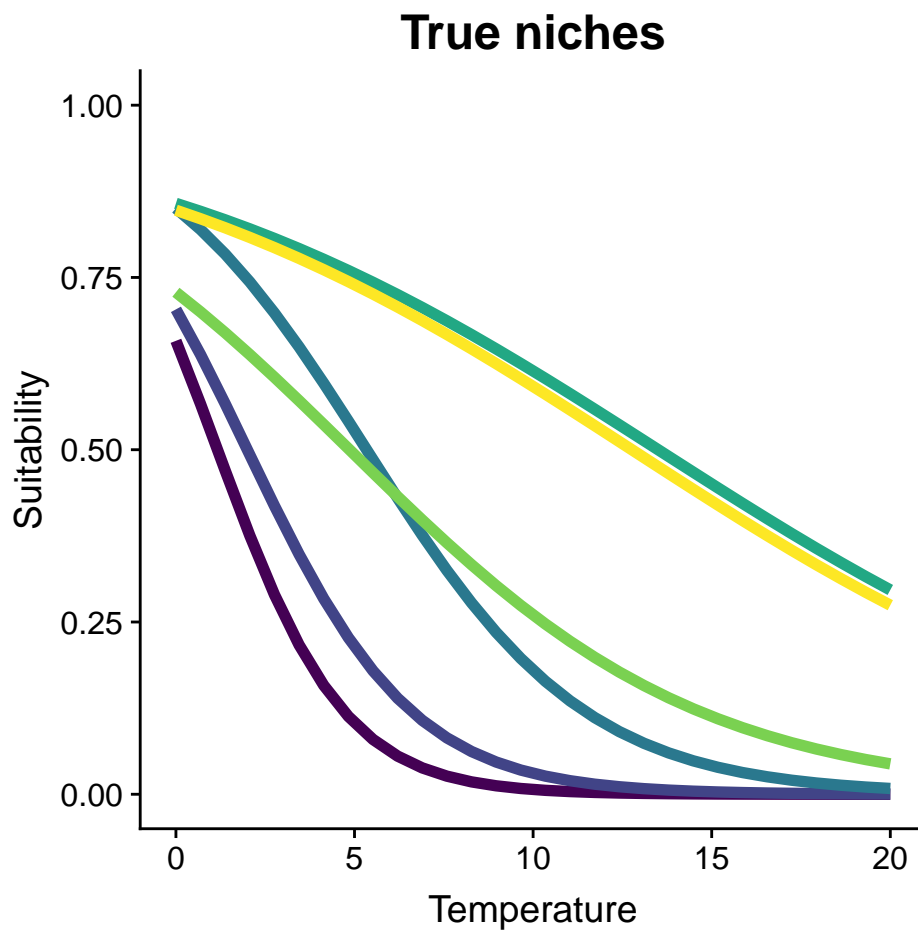
```

library(ggplot2)
library(cowplot)
library(viridis)

simul.niches <- ggplot(dat, aes(env, suitab.invlogit, colour = taxa)) +
  ylim(0, 1) +
  labs(x = "Temperature", y = "Suitability", title = "True niches") +
  geom_line(size = 2) +
  scale_color_viridis(discrete = TRUE) +
  theme(plot.title = element_text(size = 18)) +
  theme(legend.position = "none")

```

```
simul.niches
```



Plot phylogeny

```
library(ggtree)

phylog <- ggplot(phy) +
  geom_tree(size = 2, colour = "grey70") +
  geom_tree(size = 2, aes(color = label)) +
  scale_color_viridis(discrete = "TRUE") +
  theme(legend.position = "none",
        axis.title = element_blank(),
```

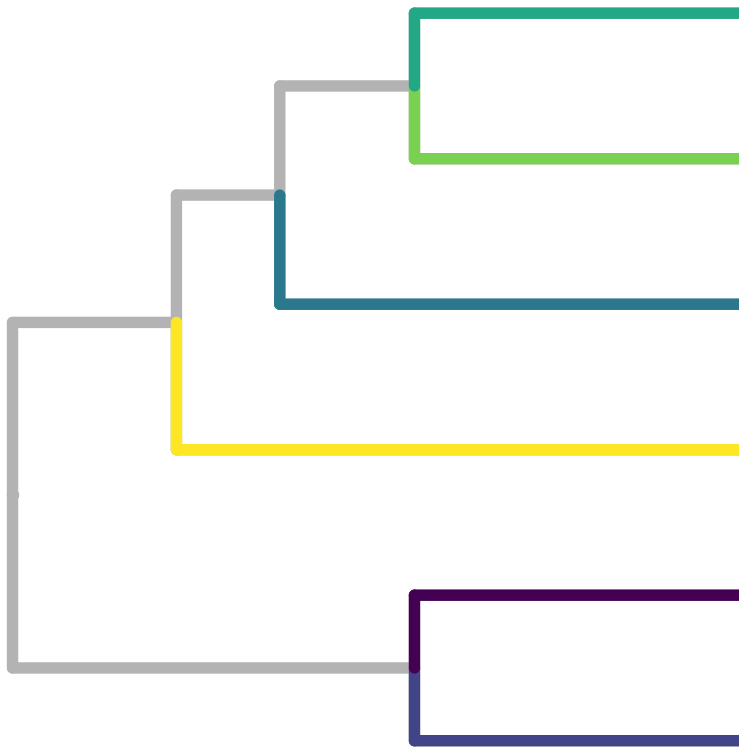
```

axis.text = element_blank(),
axis.ticks = element_blank(),
axis.line = element_blank()) +
labs(title = "Phylogeny") +
theme(plot.title = element_text(size = 18)) +
theme(plot.margin = unit(c(0.2,1,1,1), "cm"))

```

phylog

Phylogeny

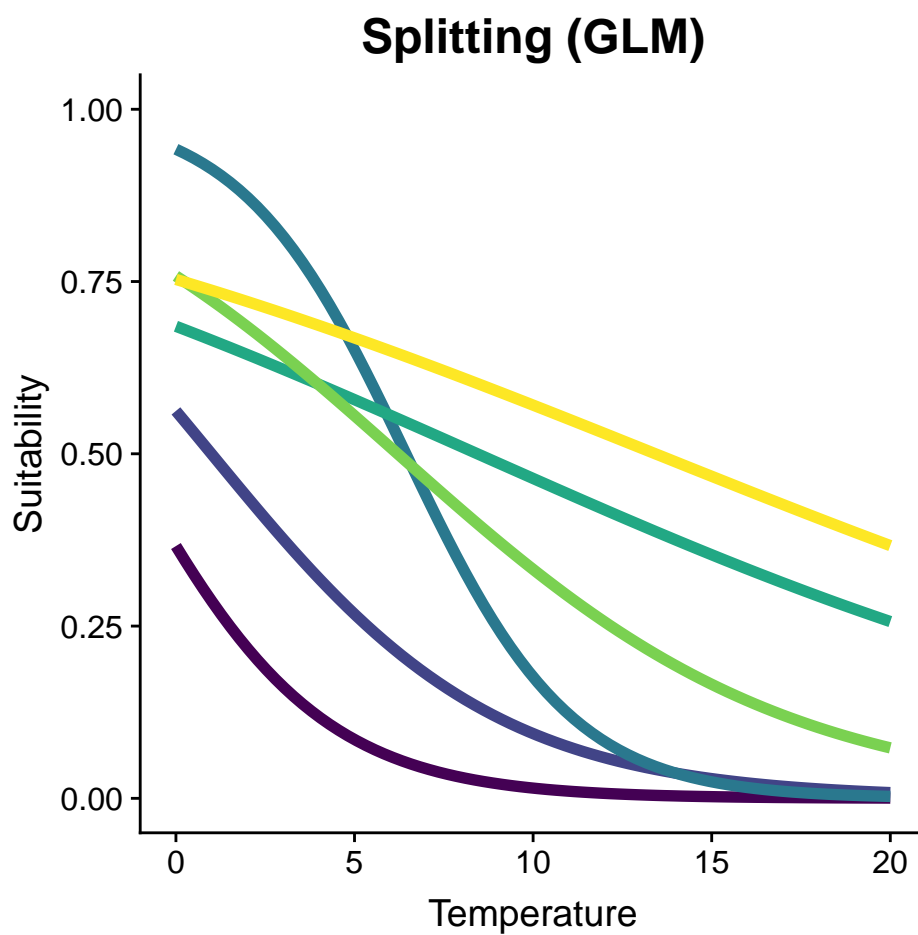


Splitting

Here we fit independent binomial generalized linear models (GLM) to each taxon.

```
split <- ggplot(dat, aes(env, presabs, colour = taxa)) +
  ylim(0, 1) +
  labs(x = "Temperature", y = "Suitability", title = "Splitting (GLM)") +
  geom_smooth(method = "glm", method.args = list(family = "binomial"), se = FALSE, size = 2)
  scale_color_viridis(discrete = TRUE) +
  theme(plot.title = element_text(size = 18)) +
  theme(legend.position = "none")
```

split



Lumping

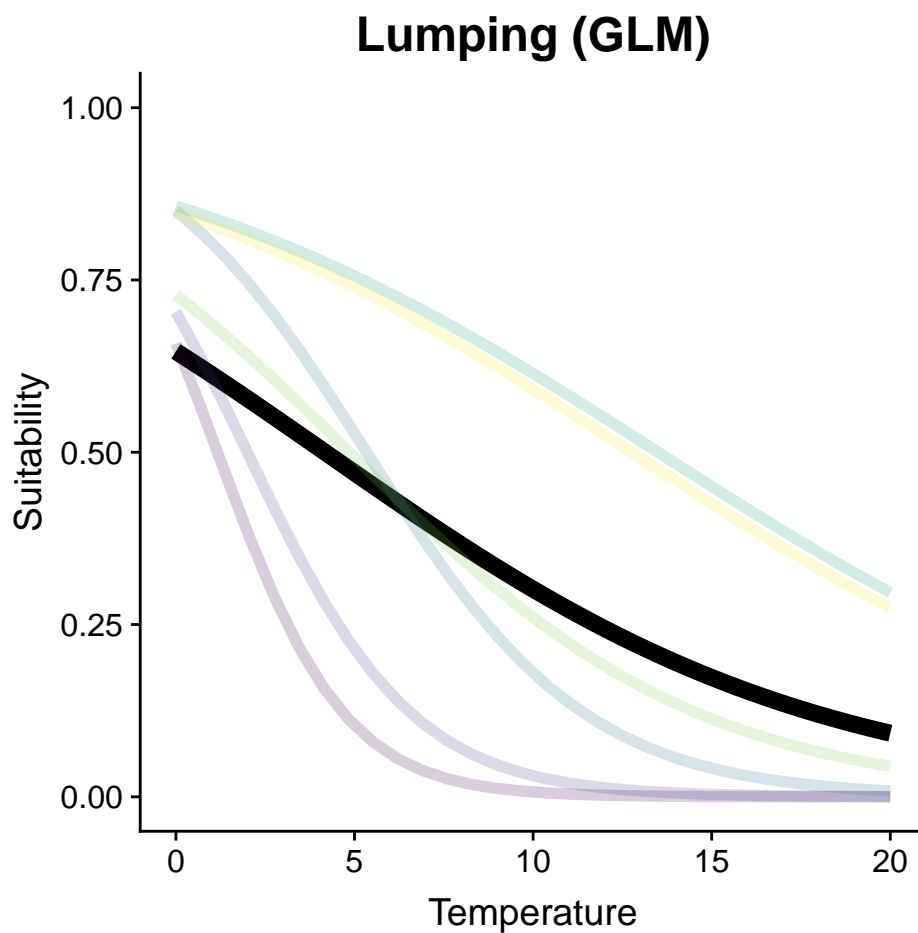
Here we fit a single binomial generalized linear model (GLM) to all taxa together.

```

lump <- ggplot(dat, aes(env, presabs)) +
  ylim(0, 1) +
  labs(x = "Temperature", y = "Suitability", title = "Lumping (GLM)") +
  geom_smooth(method = "glm", method.args = list(family = "binomial"), se = FALSE, size = 3,
    colour = "black") +
  # for comparison with real niches:
  geom_line(aes(env, suitab.invlogit, colour = taxa), size = 2, alpha = 0.2) +
  scale_color_viridis(discrete = TRUE, guide = guide_legend(override.aes = list(alpha = 1))) +
  theme(plot.title = element_text(size = 18)) +
  theme(legend.position = "none")

```

lump



Pooling (GLMM)

Here we fit a mixed effects model (GLMM) with varying intercepts and slopes, so that there is partial pooling among taxa.

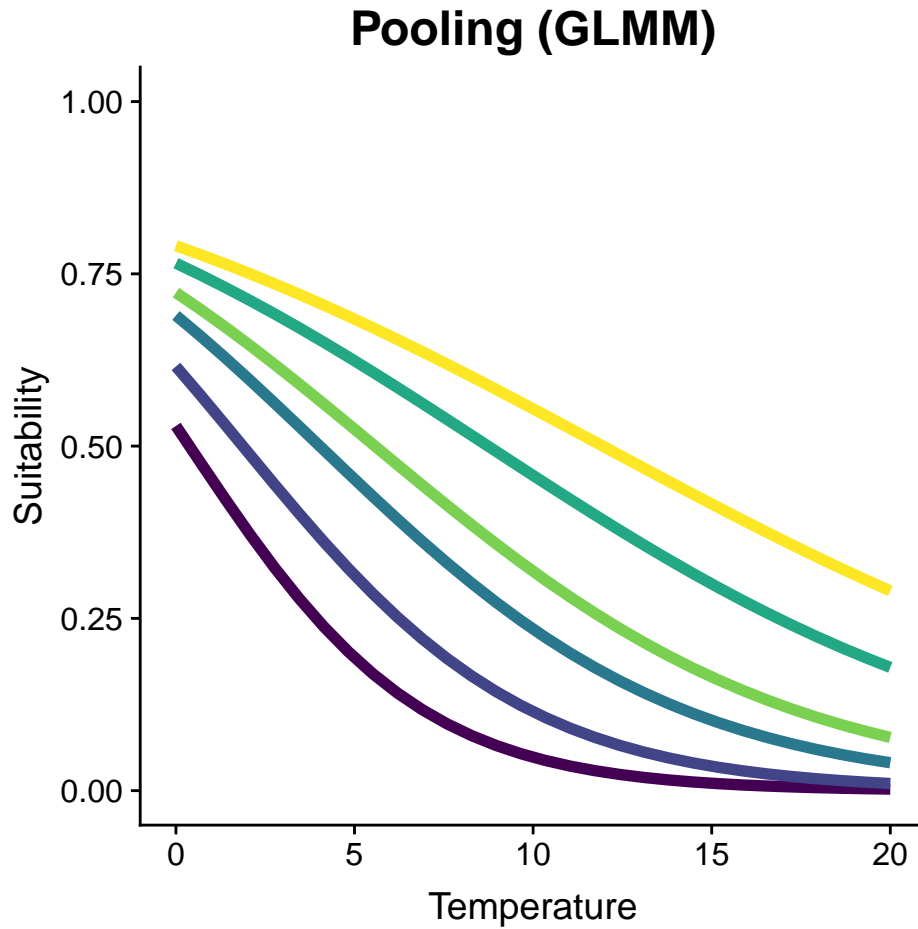
```
library(lme4)

mixed <- glmer(presabs ~ env + (1 + env | taxa), data = dat, family = binomial)
# summary(mixed)
# coef(mixed)

dat$mixedpred <- fitted(mixed, newdata = dat, type = "response")

mixedfig <- ggplot(dat, aes(env, mixedpred, colour = taxa)) +
  ylim(0, 1) +
  labs(x = "Temperature", y = "Suitability", title = "Pooling (GLMM)") +
  geom_line(size = 2) +
  scale_color_viridis(discrete = TRUE) +
  theme(plot.title = element_text(size = 18)) +
  theme(legend.position = "none")

mixedfig
```

Phylogenetic pooling (PGLMM)

Here we fit a phylogenetic generalized linear model (PGLMM) with varying intercepts and slopes, so that closely related taxa tend to have more similar niches.

```
inv.phylo <- MCMCglmm::inverseA(phy, nodes = "TIPS", scale = TRUE)
A <- solve(inv.phylo$Ainv)
rownames(A) <- rownames(inv.phylo$Ainv)

dat$phylo <- dat$taxa

library(brms)
```

```

pglmm <- brm(
  presabs ~ env + (1 + env | phylo) + (1 + env | taxa),
  data = dat,
  family = bernoulli(),
  cov_ranef = list(phylo = A),
  prior = c(
    prior(normal(0, 3), "b"),
    prior(normal(0, 3), "Intercept"),
    prior(student_t(3, 0, 3), "sd")), # sd of group random effect
  chains = 3, cores = 3, iter = 2000,
  control = list(adapt_delta = 0.96)
)

```

```

# summary(pglmm)
# plot(pglmm)
# coef(pglmm)
# pp_check(pglmm)

```

```

dat$pglmm <- fitted(pglmm, newdata = dat, scale = "response")[,1]

```

```

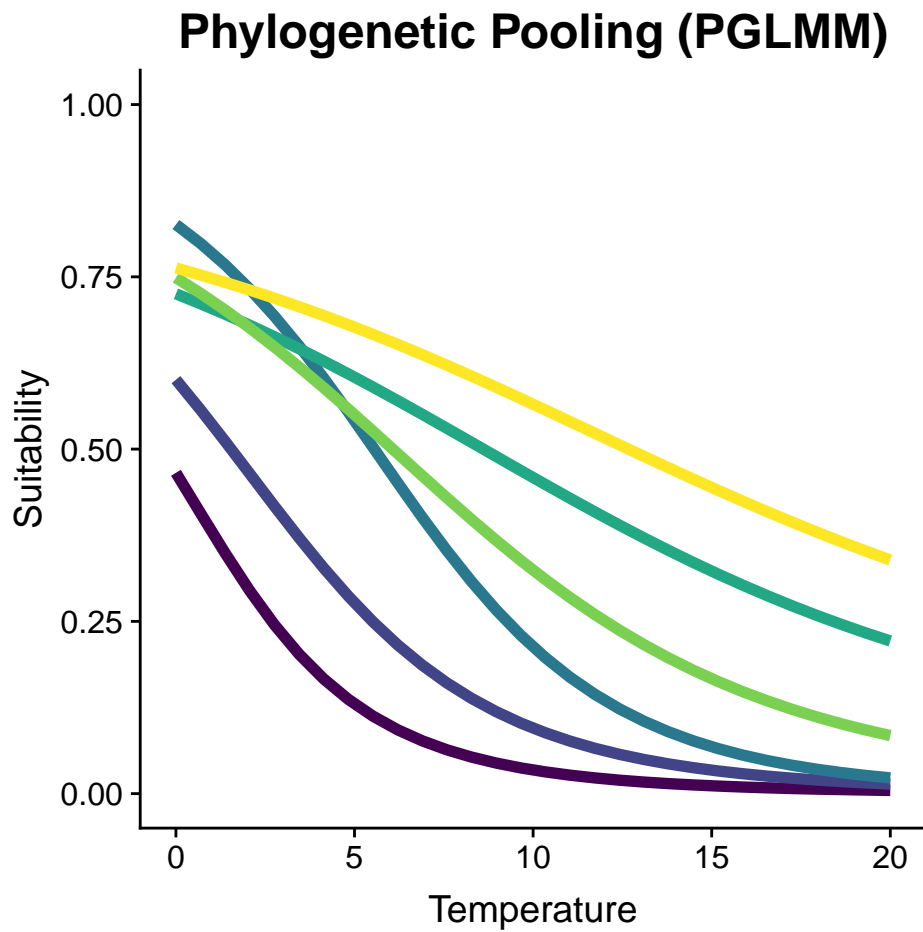
pglmmfig <- ggplot(dat, aes(env, pglmm, colour = taxa)) +
  ylim(0, 1) +
  labs(x = "Temperature", y = "Suitability", title = "Phylogenetic Pooling (PGLMM)") +
  geom_line(size = 2) +
  scale_color_viridis(discrete = TRUE) +
  theme(plot.title = element_text(size = 18)) +
  theme(legend.position = "none")

```

```

pglmmfig

```



Combined figure

```
figure <- plot_grid(simul.niches, phylog,  
                    split, lump,  
                    mixedfig, pglmmfig,  
                    nrow = 3, ncol = 2)  
  
#figure  
  
save_plot(paste0("FigureBox3", ".pdf"), figure, base_height = 11, base_width = 9)
```

References and software used

- Bates, Douglas, Martin Mächler, Ben Bolker, and Steve Walker. 2015. “Fitting Linear Mixed-Effects Models Using lme4.” *Journal of Statistical Software* 67 (1): 1–48. doi:10.18637/jss.v067.i01.
- Bürkner, Paul-Christian. 2017. “brms: An R Package for Bayesian Multilevel Models Using Stan.” *Journal of Statistical Software* 80 (1): 1–28. doi:10.18637/jss.v080.i01.
- Garnier, Simon. 2018. Viridis: Default Color Maps from 'Matplotlib'. <https://CRAN.R-project.org/package=viridis>.
- Hadfield, Jarrod D. 2010. “MCMC Methods for Multi-Response Generalized Linear Mixed Models: The MCMCglmm R Package.” *Journal of Statistical Software* 33 (2): 1–22. <http://www.jstatsoft.org/v33/i02/>.
- Paradis, E., J. Claude, and K. Strimmer. 2004. “APE: Analyses of Phylogenetics and Evolution in R Language.” *Bioinformatics* 20: 289–90.
- Pearse WD, MW Cadotte, J Cavender-Bares, AR Ives, C Tucker, S Walker & MR Helmus. 2016. A gentle introduction to Phylogenetic Generalised Linear Mixed Models. <https://cran.r-project.org/web/packages/pez/vignettes/pez-pglmm-overview.pdf>
- R Core Team. 2018. R: A Language and Environment for Statistical Computing. Vienna, Austria: R Foundation for Statistical Computing. <https://www.R-project.org/>.
- Rodríguez-Sánchez F. 2018. R code for comparing splitting, lumping, partial pooling, and phylogenetically-informed ecological niche models (version 1.1). Zenodo. <http://doi.org/10.5281/zenodo.1470855>
- Wickham, Hadley. 2009. Ggplot2: Elegant Graphics for Data Analysis. Springer-Verlag New York. <http://ggplot2.org>.
- Wilke, Claus O. 2017. Cowplot: Streamlined Plot Theme and Plot Annotations for 'Ggplot2'. <https://CRAN.R-project.org/package=cowplot>.

Xie, Yihui. 2018. Knitr: A General-Purpose Package for Dynamic Report Generation in R. <https://yihui.name/knitr/>.

Yu, Guangchuang, David Smith, Huachen Zhu, Yi Guan, and Tommy Tsan-Yuk Lam. 2017. “Ggtree: An R Package for Visualization and Annotation of Phylogenetic Trees with Their Covariates and Other Associated Data.” *Methods in Ecology and Evolution*. [doi:10.1111/2041-210X.12628](https://doi.org/10.1111/2041-210X.12628).

Details on computation environment

```
## - Session info -----
##   setting  value
##   version  R version 3.5.2 (2018-12-20)
##   os       Windows 7 x64 SP 1
##   system   x86_64, mingw32
##   ui       RTerm
##   language (EN)
##   collate  English_United Kingdom.1252
##   ctype    English_United Kingdom.1252
##   tz       Europe/Paris
##   date     2019-01-29
##
## - Packages -----
```

## package	* version	date	lib	source
## abind	1.4-5	2016-07-21	[1]	CRAN (R 3.5.0)
## ape	* 5.2	2018-09-24	[1]	CRAN (R 3.5.1)
## arm	1.10-1	2018-04-13	[1]	CRAN (R 3.5.1)
## assertthat	0.2.0	2017-04-11	[1]	CRAN (R 3.5.0)
## backports	1.1.3	2018-12-14	[1]	CRAN (R 3.5.2)
## base64enc	0.1-3	2015-07-28	[1]	CRAN (R 3.5.0)
## bayesplot	1.6.0	2018-08-02	[1]	CRAN (R 3.5.1)
## bindr	0.1.1	2018-03-13	[1]	CRAN (R 3.5.0)

##	bindrcpp	0.2.2	2018-03-29	[1]	CRAN	(R 3.5.0)
##	bridgesampling	0.6-0	2018-10-21	[1]	CRAN	(R 3.5.1)
##	brms	* 2.7.0	2018-12-17	[1]	CRAN	(R 3.5.2)
##	Brobdingnag	1.2-6	2018-08-13	[1]	CRAN	(R 3.5.1)
##	callr	3.1.1	2018-12-21	[1]	CRAN	(R 3.5.2)
##	cli	1.0.1	2018-09-25	[1]	CRAN	(R 3.5.1)
##	coda	0.19-2	2018-10-08	[1]	CRAN	(R 3.5.1)
##	codetools	0.2-16	2018-12-24	[2]	CRAN	(R 3.5.2)
##	colorspace	1.4-0	2019-01-13	[1]	CRAN	(R 3.5.2)
##	colourpicker	1.0	2017-09-27	[1]	CRAN	(R 3.5.0)
##	corpcor	1.6.9	2017-04-01	[1]	CRAN	(R 3.5.0)
##	cowplot	* 0.9.4	2019-01-08	[1]	CRAN	(R 3.5.2)
##	crayon	1.3.4	2017-09-16	[1]	CRAN	(R 3.5.0)
##	crosstalk	1.0.0	2016-12-21	[1]	CRAN	(R 3.5.0)
##	cubature	2.0.3	2018-12-18	[1]	CRAN	(R 3.5.2)
##	digest	0.6.18	2018-10-10	[1]	CRAN	(R 3.5.1)
##	dplyr	0.7.8	2018-11-10	[1]	CRAN	(R 3.5.1)
##	DT	0.5	2018-11-05	[1]	CRAN	(R 3.5.1)
##	dygraphs	1.1.1.6	2018-07-11	[1]	CRAN	(R 3.5.1)
##	evaluate	0.12	2018-10-09	[1]	CRAN	(R 3.5.1)
##	ggplot2	* 3.1.0	2018-10-25	[1]	CRAN	(R 3.5.1)
##	ggribes	0.5.1	2018-09-27	[1]	CRAN	(R 3.5.1)
##	ggtree	* 1.4.20	2018-03-10	[1]	Bioconductor	
##	glue	1.3.0	2018-07-17	[1]	CRAN	(R 3.5.1)
##	gridExtra	2.3	2017-09-09	[1]	CRAN	(R 3.5.0)
##	gtable	0.2.0	2016-02-26	[1]	CRAN	(R 3.5.0)
##	gtools	3.8.1	2018-06-26	[1]	CRAN	(R 3.5.0)
##	htmltools	0.3.6	2017-04-28	[1]	CRAN	(R 3.5.0)
##	htmlwidgets	1.3	2018-09-30	[1]	CRAN	(R 3.5.1)
##	httpuv	1.4.5.1	2018-12-18	[1]	CRAN	(R 3.5.2)

##	igraph	1.2.2	2018-07-27	[1]	CRAN	(R 3.5.1)
##	inline	0.3.15	2018-05-18	[1]	CRAN	(R 3.5.0)
##	jsonlite	1.6	2018-12-07	[1]	CRAN	(R 3.5.2)
##	knitr	1.21	2018-12-10	[1]	CRAN	(R 3.5.2)
##	labeling	0.3	2014-08-23	[1]	CRAN	(R 3.5.0)
##	later	0.7.5	2018-09-18	[1]	CRAN	(R 3.5.1)
##	lattice	0.20-38	2018-11-04	[1]	CRAN	(R 3.5.1)
##	lazyeval	0.2.1	2017-10-29	[1]	CRAN	(R 3.5.0)
##	lme4	* 1.1-19	2018-11-10	[1]	CRAN	(R 3.5.1)
##	loo	2.0.0	2018-04-11	[1]	CRAN	(R 3.5.0)
##	magrittr	1.5	2014-11-22	[1]	CRAN	(R 3.5.0)
##	markdown	0.9	2018-12-07	[1]	CRAN	(R 3.5.2)
##	MASS	7.3-51.1	2018-11-01	[1]	CRAN	(R 3.5.1)
##	Matrix	* 1.2-15	2018-11-01	[1]	CRAN	(R 3.5.1)
##	matrixStats	0.54.0	2018-07-23	[1]	CRAN	(R 3.5.1)
##	MCMCglmm	2.26	2018-07-03	[1]	CRAN	(R 3.5.1)
##	mime	0.6	2018-10-05	[1]	CRAN	(R 3.5.1)
##	miniUI	0.1.1.1	2018-05-18	[1]	CRAN	(R 3.5.0)
##	minqa	1.2.4	2014-10-09	[1]	CRAN	(R 3.5.0)
##	munsell	0.5.0	2018-06-12	[1]	CRAN	(R 3.5.1)
##	mvtnorm	1.0-8	2018-05-31	[1]	CRAN	(R 3.5.0)
##	nlme	3.1-137	2018-04-07	[1]	CRAN	(R 3.5.1)
##	nloptr	1.2.1	2018-10-03	[1]	CRAN	(R 3.5.1)
##	pillar	1.3.1	2018-12-15	[1]	CRAN	(R 3.5.2)
##	pkgbuild	1.0.2	2018-10-16	[1]	CRAN	(R 3.5.1)
##	pkgconfig	2.0.2	2018-08-16	[1]	CRAN	(R 3.5.1)
##	plyr	1.8.4	2016-06-08	[1]	CRAN	(R 3.5.0)
##	prettyunits	1.0.2	2015-07-13	[1]	CRAN	(R 3.5.0)
##	processx	3.2.1	2018-12-05	[1]	CRAN	(R 3.5.2)
##	promises	1.0.1	2018-04-13	[1]	CRAN	(R 3.5.0)

##	ps	1.3.0	2018-12-21	[1]	CRAN	(R 3.5.2)
##	purrr	0.2.5	2018-05-29	[1]	CRAN	(R 3.5.1)
##	R6	2.3.0	2018-10-04	[1]	CRAN	(R 3.5.1)
##	Rcpp	* 1.0.0	2018-11-07	[1]	CRAN	(R 3.5.1)
##	reshape2	1.4.3	2017-12-11	[1]	CRAN	(R 3.5.1)
##	rlang	0.3.1	2019-01-08	[1]	CRAN	(R 3.5.2)
##	rmarkdown	1.11	2018-12-08	[1]	CRAN	(R 3.5.2)
##	rsconnect	0.8.13	2019-01-10	[1]	CRAN	(R 3.5.2)
##	rstan	2.18.2	2018-11-07	[1]	CRAN	(R 3.5.1)
##	rstantools	1.5.1	2018-08-22	[1]	CRAN	(R 3.5.1)
##	scales	1.0.0	2018-08-09	[1]	CRAN	(R 3.5.1)
##	sessioninfo	1.1.1	2018-11-05	[1]	CRAN	(R 3.5.1)
##	shiny	1.2.0	2018-11-02	[1]	CRAN	(R 3.5.1)
##	shinyjs	1.0	2018-01-08	[1]	CRAN	(R 3.5.0)
##	shinystan	2.5.0	2018-05-01	[1]	CRAN	(R 3.5.0)
##	shinythemes	1.1.2	2018-11-06	[1]	CRAN	(R 3.5.1)
##	StanHeaders	2.18.0-1	2018-12-13	[1]	CRAN	(R 3.5.2)
##	stringi	1.2.4	2018-07-20	[1]	CRAN	(R 3.5.1)
##	stringr	1.3.1	2018-05-10	[1]	CRAN	(R 3.5.0)
##	tensorA	0.36.1	2018-07-29	[1]	CRAN	(R 3.5.1)
##	threejs	0.3.1	2017-08-13	[1]	CRAN	(R 3.5.0)
##	tibble	2.0.1	2019-01-12	[1]	CRAN	(R 3.5.2)
##	tidyr	0.8.2	2018-10-28	[1]	CRAN	(R 3.5.1)
##	tidyselect	0.2.5	2018-10-11	[1]	CRAN	(R 3.5.1)
##	viridis	* 0.5.1	2018-03-29	[1]	CRAN	(R 3.5.0)
##	viridisLite	* 0.3.0	2018-02-01	[1]	CRAN	(R 3.5.0)
##	withr	2.1.2	2018-03-15	[1]	CRAN	(R 3.5.0)
##	xfun	0.4	2018-10-23	[1]	CRAN	(R 3.5.1)
##	xtable	1.8-3	2018-08-29	[1]	CRAN	(R 3.5.1)
##	xts	0.11-2	2018-11-05	[1]	CRAN	(R 3.5.1)


```
## yaml                2.2.0    2018-07-25 [1] CRAN (R 3.5.1)
## zoo                 1.8-4     2018-09-19 [1] CRAN (R 3.5.1)
##
## [1] C:/Users/FRS/Documents/R/win-library/3.5
## [2] C:/R/R-3.5.2/library
```