Biology 559R: Introduction to Phylogenetic Comparative Methods

Topics for this week (Mar 10 & 12):
• Ancestral reconstructions and diversification:
  Binary-State Speciation and Extinction (BiSSE) models.
What can explain differences in diversification rates?

What can explain differences in diversification rates?

- **Causal or deterministic:** Emergence of phenotypic innovation (adaptive or not) that is associated with speciation or extinction (e.g., reproductive isolation, adaptive radiation, sexual selection).

- **Causal or deterministic:** Non-biological factors that are associated with the process of speciation or extinction (e.g., climate change, geographic isolation, habitat destruction).

- **Causal or deterministic:** External biological factors that are associated with the process of speciation or extinction (e.g., effective predators and parasites).

- **Random** fluctuations associated with persistence or extinction of species with a clade of lineage that we are studying (e.g. population dynamic, genetic drift).
Speciation versus Extinction Rates

• Two main parameters allow us to understand the process of diversification.

  Speciation rate (increase in diversity) = b-birth rate or lambda (λ) parameter
  Extinction rate (loss of diversity) = d-death rate or mu (μ) parameter

• The balance between these two rates can explain differences in the diversification between lineages.

• The relationship between these parameters can be also use to characterize diversification including:

  Net diversification rate (r): λ − µ  or  Relative extinction rate (ε): μ / λ
• Remember, the Yule process (pure birth – no extinction) versus birth-death process when we simulated trees.

• The goal of most analyses that deal with diversification estimate the speciation and extinction rates to address current and past diversity.

• However, extinction rates should not be estimated in the absence of fossil data.

Figure 4. Contrasting effects of lineage-specific increases and decreases in the speciation rate (λ) on the shape of lineage-through-time (LTT) curves. (A) Expected LTT curve under a pure-birth process (μ = 0) with λ constant among lineages. (B) Expected LTT curve when a single lineage undergoes a major decrease in λ. (C) Expected lineage through time plot when a single lineage undergoes a major increase in λ. The rapid rise in the number of lineages toward the present leads to estimates of high ε, even when extinction is not present. The effects of a single rate decrease should be statistically indistinguishable from a constant-rate process. However, a rate increase can exert a large effect on the shape of LTT curves, because all descendants of the high-rate lineage inherit an elevated λ and thus contribute disproportionately to clade diversity. The slope of the LTT curve approaches and, given sufficient time, becomes equal to the new (elevated) λ.

Some tree terminology when addressing diversification

Fig. 1. Stem group and crown group age. The age of the stem group is the time of divergence of the clade from its sister taxon. The age of the crown group is the time of the deepest bifurcation within the crown group. Solid lines represent living species; dotted lines represent extinct species.

• We need our time calibrated phylogeny (chronogram) the we can derive a well-support maximum likelihood estimator (MLE)

\[ \hat{r} = \hat{\lambda} = \log(n)/t \]

\[ \hat{r} = \hat{\lambda} = [\log(n) - \log 2]/t \]

\( n \) is the number of species at time \((t)\)

Fig. 1. Stem group and crown group age. The age of the stem group is the time of divergence of the clade from its sister taxon. The age of the crown group is the time of the deepest bifurcation within the crown group. Solid lines represent living species; dotted lines represent extinct species.
Determining Speciation Rate

- We need our time calibrated phylogeny (chronogram) the we can derive a well-support maximum likelihood estimator (MLE)

\[ \hat{r} = \hat{\lambda} = \frac{\log(n)}{t} \]

\[ \hat{r} = \hat{\lambda} = \left[ \log(n) - \log 2 \right]/t \]

Yet, there is clear that \( \mu \) (extinction rate) is neglected or needs to be estimate from branching pattern in our phylogeny usually from lineage-through time plots (LTT)

**Fig. 1.** Stem group and crown group age. The age of the stem group is the time of divergence of the clade from its sister taxon. The age of the crown group is the time of the deepest bifurcation within the crown group. Solid lines represent living species; dotted lines represent extinct species.
• We can estimate the rate of extinction as a function of the speciation rate

Discrete Character Evolution and Species Diversification

• A new trend in comparative methods has been the progressive incorporation of correlative association between character evolution and diversification (speciation and extinction) rates.

• The most well-known methods focus on discrete traits (mostly binary 0-no, 1-yes) and on how rates for transition between character states are associated with diversification.

• For example, the transition from 0-absent to 1-present has resulted in significant increased in diversification (an example of adaptive radiation).

• Most models are based on the continuous-time dependent Markov process (Q-matrix or cost of change between character states) reflecting transition rates between states.
The BiSSE model

• The Binary-State Speciation and Extinction (BiSSE) model allows to estimate simultaneously both character evolution and diversification rates.

• The BiSSE model allow to calculate rates of speciation and extinction associate to each character state.

• This model used a likelihood estimation and compares the more complex model (e.g., rates of transition between character states and speciation-extinction rates) versus nested and more simple models where one or more parameters are fixed.
Evaluating the BiSSE model

• Three basic approaches allow us to compare alternative models based on the BiSSE method:

1) Comparing Likelihood scores: This is based on finding the best model that maximizes the likelihood (probability of true) of the data given the proposed BiSSE model.

It uses the likelihood-ratio test (LRT) if models are nested:

\[
\text{Likelihood Ratio} = 2 \ast (\ln L_{\text{complex model}} - \ln L_{\text{constraint model}})
\]

It assumes that the LRT has can be approximated by a \( \chi^2 \) distribution with degrees of freedom (df) determined by the difference in free parameters between the complex (full) and constraint model.
Evaluating the BiSSE model

• Three basic approaches allow us to compare alternative models based on the BiSSE method:

1) Comparing Likelihood scores: This is based on finding the best model that maximizes the likelihood (probability of true) of the data given the proposed BiSSE model.

For non-nested models, you can use the Akaike Information Criterion (AIC), where:

\[ AIC = 2k - 2\ln L \]

and the k parameters is the number of parameters estimated in the model.

Also you can use the sample size corrected such as AICc

*** Like before, the best model has the lowest AIC or AICc scores
Three basic approaches allow us to compare alternative models based on the BiSSE method:

2) **Bayesian model estimation** based on prior information and proposed model. The parameters are estimated using sampling approaches such as MCMC. We wait until the chains become stationary.

3) **Parametric simulations** that allow the construction of an statistic from which we can compare our estimated parameters to determine its likelihood. For example, simulate data (e.g., traits and phylogenies) that we can use fit complex and constraint models.

However, we should simulate our data under most simpler model. We will obtain a distribution of the frequency of parameters observed and we can compare with those estimated using our empirical data.
Diversification Analysis using ‘diversitree’

• We are going to use our an specialized R-package on BiSSE and derived models:

```r
library(diversitree)
```

• This package focus on analyzing diversification and character evolution simultaneously. The methods implemented includes:

**BiSSE (Binary State Speciation and Extinction)**; Maddison et al. 2007: Syst. Biol. 56: 701)

**MuSSE (Multiple State Speciation and Extinction)**

**QuaSSE (Quantitative State Speciation and Extinction)**; FitzJohn 2010: Syst. Biol. 59: 619),

**GeoSSE (Geographic State Speciation and Extinction)**; Goldberg et al. 2011: Syst. Biol. 60: 451)

**BiSSE-ness** (Magnuson-Ford and Otto 2012: Am. Nat.)
Diversification Analysis using ‘diversitree’

• Make a working directory (e.g., BiSSE_analyses) and select it as your working.

R top menus: Misc>Change Working Directory (select the directory that has our file)

```
setwd("/Users/jcsantos/Desktop/R_class_winter_2015_home/0_Bio559R_course_final_files/week_10/data")
```

• We need to download these files from the course website into our working directory:

```
bird_data_pruned.txt
bird_pruned_MB.newick
```

• read ‘ape’, ‘geiger’ and ‘phytools’ packages

```
library(ape)
library(geiger)
library(diversitree)
```

• Load our trees and data from last week and check concordance:

```
bird_pruned_tree <- read.tree("bird_pruned_MB.newick")
bird_pruned_tree
birds_traits_data <- read.table("bird_data_pruned.txt", header = TRUE, sep = "\t")
birds_traits_data
```
Diversification Analysis using ‘diversitree’

• Ancestral reconstruction for binary discrete traits. We are going to use only migration.

```r
birds_migration_temp <- as.data.frame(birds_traits_data$Migration) # Select this binary
data and make it a vector
birds_migration_temp$species <- birds_traits_data$Genus_Species
birds_migration_temp
```

• Eliminate incomplete cases and make data frame

```r
birds_migration_data <- birds_migration_temp[complete.cases(birds_migration_temp),]
row.names(birds_migration_data) <- birds_migration_data$species
names(birds_migration_data) <- c("migration", "genus_species")
birds_migration_data
```

```
#                          migration        genus_species
# Struthio_camelus        No              Struthio_camelus
# Dromaius_novaehollandiae No              Dromaius_novaehollandiae
# Apteryx_owenii          No              Apteryx_owenii
# Apteryx_haastii         No              Apteryx_haastii
# Apteryx_australis       No              Apteryx_australis
# Nothoprocta_perdicaria  No              Nothoprocta_perdicaria
```
Diversification Analysis using ‘diversitree’

• Prepare the data as binary

  # make factors to characters

  birds_migration_data$migration <- as.character(birds_migration_data$migration)

  # make data truly binary (0-no migratory and 1-migratory)

  birds_migration_data$migration[birds_migration_data$migration == "No"] <- "0"
  birds_migration_data$migration[birds_migration_data$migration == "Yes"] <- "1"

  birds_migration_data

• Use the 'name.check' function to determine if we have concordance

  name.check (bird_pruned_tree, birds_migration_data) # we check the concordance between a data file and a phylogenetic tree.
  # NOT CONCORDANT
  # Provides a list of species in tree with no data ($tree_not_data)
Diversification Analysis using ‘diversitree’

• Use the 'name.check' function to determine if we have concordance

name.check (bird_pruned_tree, birds_migration_data) # we check the concordance between a data file and a phylogenetic tree.
# NOT CONCORDANT
# Provides a list of species in tree with no data ($tree_not_data)

	$tree_not_data
[1] "Aegithalos_caudatus" "Aethopyga_zipara" "Aplonis_phoenicu" "Amphispiza_bilineata" "Anas_platyrhynchos"
[8] "Aythya_ferina" "Emberiza_citrinella" "Emberiza_cochlearia" "Eremophila_alpestris" "Erithacus_rubecula"
[15] "Falco_tinnunculus" "Myioborus_tricolor" "Phylloscopus_colybita" "Phytotoma_rara" "Pinicola_enucleator"
[22] "Sialia_mexicana" "Sialia_citrea" "Sturnus_vividus" "Troglodytes_troglodytes" "Turdus_merula"
[29] "Tyrannus_melancholicus" "Upupa_epops" "Zenaida_macroura" "Zenaida_reichenbachii" "Zonotrichia_acephala"

$tree_not_tree
character(0)

• We make concordant need to prepare our data using the function 'treedata'

birds_migration <- treedata(bird_pruned_tree, birds_migration_data)
birds_migration$phy # a class phylo
birds_migration$data # a matrix

# We are going to prepare our data for analyses:

birds_migration_phy <- birds_migration$phy
birds_migration_dat <- as.numeric(birds_migration$data[,1])
names(birds_migration_dat) <- birds_migration$data[,2]
birds_migration_dat_matrix <- as.matrix(birds_migration_dat)
Diversification Analysis using ‘diversitree’

• Let's start with the most simple BiSSE analyses. A constant rate of speciation and extinction (i.e., fitting a birth-death model) through the chronogram.

• This model assumes that the net diversification (birth - death) does not change over the lineage history or it is associated with any phenotype.
Diversification Analysis using ‘diversitree’

• For most diversification analyses, we need to estimate the most complex model and then a more simpler model by forcing some parameters to be constants.

• Then, we compare model fit between the complex and simple models.

• For the basic birth-death model, we are looking for significant birth (speciation) versus death (extinction) rates.

Step 1: Define a likelihood function for the phylogeny.

birds_migration_bd_full.lik <- make.bd(birds_migration_phy)
birds_migration_bd_full.lik

# Constant rate birth-death likelihood function:
#   * Parameter vector takes 2 elements:
#     - lambda, mu
#   * Function takes arguments (with defaults)
#     - pars: Parameter vector
#     - condition.surv [TRUE]: Condition likelihood on survival?
#     - intermediates [FALSE]: Also return intermediate values?
#   * Phylogeny with 399 tips and 398 nodes
#   - Taxa: Nothoprocta_perdicaria, Apteryx_australis, Apteryx_haastii,
#   * Reference:

argnames(birds_migration_bd_full.lik) # function that gives the name of parameters
# [1] "lambda" "mu" → these are the speciation-lambda and extinction-mu rates
For specific values, we can use our likelihood function and estimate model likelihood scores:

Step 2: we can estimate the likelihood for a given set of parameter values using the likelihood function that we estimated for our tree.

# pure-birth: c(0.5, 0) --> lambda = 0.5 and extinction = 0 (Yule process)

```r
birds_migration_bd_full.lik(c(0.5, 0))
# [1] -3178.799
```

# birth-death values: c(0.2, 0.1)

```r
birds_migration_bd_full.lik(c(0.2, 0.1))
# [1] -63.90782
```

For example, we can compare both likelihood scores and we want the highest (less negative) score. Then, we can conclude that the birth-death model with lambda = 0.2 and extinction = 0.1 is much better.
Diversification Analysis using ‘diversitree’

• However, we are more interested in the parameters that maximizes the model score (i.e., its maximum likelihood estimator)

Step 3: We can find the MLE (maximum likelihood estimator) that will select the best values for lambda and mu that maximize the likelihood score using `find.mle()`.

# Notice: you can also use to get starting points for estimation

`starting.point.bd(birds_migration_phy, yule=FALSE)`

```
#   lambda         mu
# 0.04057479 0.00000000
```

`parameters_bd <- c(0.2, 0.1)`

`birds_migration_bd_fit_mle <- find.mle(birds_migration_bd_full.lik, parameters_bd)`

```
# $par
#           lambda             mu
# $ 4.836804e-02   4.944044e-06
# $lnLik
# [1] 312.7964
# $counts
# [1] 21
# $code
# [1] 2
```
Diversification Analysis using ‘diversitree’

- Let’s explore the results of the MLE of this function:

```r
names(birds_migration_bd_fit_mle)
# [1] "par"   "lnLik"   "counts"   "code"   "gradient"   "method"   "func.class"

birds_migration_bd_fit_mle$par # gives lambda and mu
birds_migration_bd_fit_mle$lnLik # gives the lnLik (score)
birds_migration_bd_fit_mle$count # The number of function evaluations
birds_migration_bd_fit_mle$code # Convergence code and 0 is preferred

coef(birds_migration_bd_fit_mle) # gives lambda and mu
logLik(birds_migration_bd_fit_mle) # gives the log Lik. 312.7964 (df=2)
AIC(birds_migration_bd_fit_mle)   # -621.5928 score
```
Diversification Analysis using ‘diversitree’

• We can now estimate the net diversification rate (i.e., $r = \lambda - \mu$)

```r
birds_migration_bd_fit_mle_r <- birds_migration_bd_fit_mle$par[1] -
birds_migration_bd_fit_mle$par[2]
birds_migration_bd_fit_mle_r <- birds_migration_bd_fit_mle$par['lambda'] -
birds_migration_bd_fit_mle$par['mu'] # the same process
```

# 0.0483631

• We also can estimate the ratio between speciation and extinction

```r
birds_migration_bd_fit_mle$par[1]/birds_migration_bd_fit_mle$par[2]
```

# 9783.093

Notice this value is very large ($\lambda$ is almost 10000 times larger than $\mu$)
• We can now estimate the net diversification rate (i.e., \( r = \lambda - \mu \))

```r
birds_migration_bd_fit_mle_r <- birds_migration_bd_fit_mle$par[1] - birds_migration_bd_fit_mle$par[2]
birds_migration_bd_fit_mle_r <- birds_migration_bd_fit_mle$par['lambda'] - birds_migration_bd_fit_mle$par['mu'] # the same process
```

```
# 0.0483631
```

• We also can estimate the ratio between speciation and extinction

```r
birds_migration_bd_fit_mle$par[1]/birds_migration_bd_fit_mle$par[2]
```

```
# 9783.093
```

**Notice** this value is very large (\( \lambda \) is almost 10000 times larger than \( \mu \))
Diversification Analysis using ‘diversitree’

- Defining constrain (simpler) models is necessary before we can compare to our full model. We use the function ‘constrain’ to create new function that satisfies the condition

  `constrain (lik function, parameters to constrain defined by par_A '~' par_B or a value)`

```r
bird_mu_0.lik <- constrain(birds_migration_bd_full.lik, mu ~ 0) # pure birth, extinction = 0
argnames(bird_mu_0.lik) # [1] "lambda" --> only lambda is a free parameter

bird_lambda_equal_mu.lik <- constrain(birds_migration_bd_full.lik, lambda ~ mu)
argnames(bird_lambda_equal_mu.lik) # [1] "mu" --> only mu is a free parameter
```
Diversification Analysis using ‘diversitree’

• Let's evaluate constrain functions

```r
birds_migration_mu_0_mle <- find.mle(bird_mu_0.lik, 0.1) # 0.1 is an starting parameter for lambda
birds_migration_mu_0_mle

# $par
#    lambda
# 0.04057479

# $lnLik
# [1] 319.2956

# $counts
# [1] 8

# $code
# [1] 1

logLik(birds_migration_mu_0_mle) # 'log Lik.' 319.2956 (df=1)
```
Diversification Analysis using ‘diversitree’

• Let's evaluate constrain functions

```r
# Let's evaluate constrain functions

everything <- sample(1:100, 100, replace = TRUE)

b <- birds_migration_lambda_equal_mu_mle <- find.mle(bird_lambda_equal_mu.lik, 0.1) # 0.1 is an
starting parameter for mu
birds_migration_lambda_equal_mu_mle

# $par
#   mu
# 0.1

# $lnLik
# [1] 221.9229

# $counts
# [1] 0

# $code
# [1] 1
```
Diversification Analysis using ‘diversitree’

• Model comparison using ANOVA

# extinction constraint is null

anova(birds_migration_bd_fit_mle, mu_0=birds_migration_mu_0_mle)

#  Df lnLik AIC  ChiSq Pr(>|Chi|)
# full  2 312.8 -621.59
# mu_0  1 319.3 -636.59  -12.998  1

Notice: that the chi-square is not valid. However, see the AIC difference > 10 and the best model (full) has lowest AIC. Therefore, speciation is higher than extinction.

# speciation and extinction equal

anova(birds_migration_bd_fit_mle, lambda_equal_mu=birds_migration_lambda_equal_mu_mle)

#  Df lnLik  AIC  ChiSq Pr(>|Chi|)
# full  2 312.80 -621.59
# lambda_equal_mu  1 221.92 -441.85  181.75  < 2.2e-16 ***
# ---
# Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

We reject that lambda and mu are equal
• Let's try character evolution using the basic Mk2 as an example of Mk-n Models of character evolution. This approaches replicates the ace function in ape. However, it also includes:

(1) alternative root treatments are possible,

(2) easier to tweak parameter combinations through constrain

(3) run both MCMC and MLE fits to parameters.

Three flavors:

**binary:** make.mk2(tree, states, strict=TRUE, control=list())

**k states:** make.mkn(tree, states, k, strict=TRUE, control=list())

**k states ordered:** make.mkn.meristic(tree, states, k, control=list())
Trait Evolution under Mk2 model in ‘diversitree’

• Preparing data for binary

```r
birds_migration_phy
birds_migration_dat_df <- as.data.frame(birds_migration_dat)  # make data frame
birds_migration_dat_df$species_name <- rownames(birds_migration_dat_df)  # crate column with species names
birds_migration_dat_ordered <- birds_migration_dat_df[birds_migration_phy$tip.label,]  # order data based on tree label order
birds_migration_dat_bin <- birds_migration_dat_ordered[,1]  # get vector of binary trait
names(birds_migration_dat_bin) <- rownames(birds_migration_dat_ordered)  # name elements of binary trait by species
```
Trait Evolution under Mk2 model in ‘diversitree’

• Prepare the full Mk-2 model comparison. Notice that we are not estimating diversification:

```r
# FULL MODEL: get the likelihood function
birds_migration_mk2_full.lik <- make.mk2(birds_migration_phy, birds_migration_dat_bin)
argnames(birds_migration_mk2_full.lik)

# [1] "q01"  "q10" this indicated the free parameters q01 (non-migratory to migratory)
#                                                    q10 (migratory to non-migratory)

# define constrain equal (q01 = q10) versus different rates
migratory_contratin.lik <- constrain(birds_migration_mk2_full.lik, q01 ~ q10)
argnames(migratory_contratin.lik) # [1] "q10"

# evaluate models:

birds_migration_mke_full_mle <- find.mle(birds_migration_mk2_full.lik, c(0.2, 0.1)) # q01 = 0.2, q10 = 0.1 are starting value
birds_migration_mke_full_mle

# $par
#      q01     q10
# 0.00645963 0.01744694
# $lnLik
# [1] -193.3988
# $counts
# [1] 82
# $convergence
# [1] 0 ← did converge code "0" is usually good (more info ?find.mle)
```
• Prepare the constrain Mk-2 model comparison

```r
birds_migration_mke_constrain_mle <- find.mle(migratory_contratin.lik, 0.1) # q01 = q10 = 0.1 is a starting value
birds_migration_mke_constrain_mle

# $par
#       q10
# 0.008105469

# $lnLik
# [1] -199.2046

# $counts
# [1] 36

# $convergence
# [1] 0 ← did converge code "0" is usually good (more info ?find.mle)
```

Trait Evolution under Mk2 model in ‘diversitree’
Trait Evolution under Mk2 model in ‘diversitree’

• Compare models both Mk2 models

```r
anova(birds_migration_mke_full_mle, q01_equal_q10=birds_migration_mke_constrain_mle)
```

```
# Df  lnLik  AIC  ChiSq  Pr(>|Chi|)
# full     2 -193.40 390.80
# q01_equal_q10     1 -199.21 400.41  11.612 0.0006554 ***
# ---
# Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
```

# We conclude that q01 and q10 are different and q10 > q01 (it is easier to become
# a non-migratory bird from a migratory state.

• We can estimate the likelihood that the states at internal nodes in the phylogeny using the
function: asr.marginal

```r
?asr.marginal
```

```r
birds_migration_mke_anc.states <- asr.marginal(birds_migration_mk2_full.lik,
birds_migration_mke_full_mle$par)
birds_migration_mke_anc.states_t <- t(birds_migration_mke_anc.states)
# Transposition for plotting
```
Trait Evolution under Mk2 model in `diversitree`

- Plot ancestral reconstructions for each node

```r
plot(birds_migration_phy, no.margin=TRUE, cex=0.5, label.offset=4, type = "fan")
tip_colors <- rep('blue', times=length(birds_migration_dat_bin)) # we are going to create a vector and consider blue -- no migratory
tip_colors[birds_migration_dat_bin == 1] <- 'red' # assign color red to migratory birds
tiplabels(bg=tip_colors, pch=21, adj=2.5) # Plot the tip labels on tree
nodelabels(pie=birds_migration_mke_anc.states_t, piecol=c("blue","red"), cex=0.12)
```
Trait Evolution under Mk2 model in ‘diversitree’

- Plot ancestral reconstructions for each node
Prepare BiSSE model comparison. Remember BiSSE parameters:

- $\lambda_0$ → speciation rate associated to state 0 -- no migration
- $\lambda_1$ → speciation rate associated to state 1 – migration
- $\mu_0$ → extinction rate associated to state 0 -- no migration
- $\mu_1$ → extinction rate associated to state 1 -- migration
- $q_{01}$ → transition from 0 -- no migration to 1 – migration
- $q_{10}$ → transition from 1 -- migration to 0 -- no migration
• Let's define the full likelihood BiSSE model and we can provide starting values for the likelihood search for more complicated analyses (like this one).

```r
# full BiSSE Model

birds_migration_BiSSE_full.lik <- make.bisse(birds_migration_phy, birds_migration_dat_bin)
argnames(birds_migration_BiSSE_full.lik)

# "lambda0" "lambda1" "mu0" "mu1" "q01" "q10" → we can use these to define constrain models

# get the starting values

starting_values_birds_migration <- starting.point.bisse(birds_migration_phy)
starting_values_birds_migration

# lambda0   lambda1   mu0    mu1    q01    q10
# 0.040574788 0.040574788 0.00000000 0.00000000 0.008114958 0.008114958
```
Trait Evolution under BiSSE model in ‘diversitree’

• Find the MLE for the full model

```r
birds_migration_BiSSE_full_mle <- find.mle(birds_migration_BiSSE_full.lik,
starting_values_birds_migration)
birds_migration_BiSSE_full_mle

# $par
#    lambda0    lambda1     mu0     mu1     q01     q10
# 0.03296855 0.05208791 0.00000000 0.00000000 0.00388844 0.02504977

# $lnLik
# [1] -1856.445

# $counts
# [1] 304

# $convergence
# [1] 0  # evidence of convergence
```
• Define different constrain models

```r
# same speciation rate equal (lambda0 = lambda1)

starting_values_birds_migration[2:6] # less starting parameters

# lambda1   mu0   mu1   q01   q10
# 0.040574788 0.000000000 0.000000000 0.008114958 0.008114958

migratory_constrain_speciation_rate_BiSSE.lik <- constrain(birds_migration_BiSSE_full.lik, lambda0 ~ lambda1)
constratin_speciation_rate_BiSSE_mle <- find.mle(migratory_constrain_speciation_rate_BiSSE.lik, starting_values_birds_migration[2:6])
constratin_speciation_rate_BiSSE_mle

# $par
# lambda1   mu0   mu1   q01   q10
# 4.059865e-02 3.272882e-05 8.947200e-06 6.441251e-03 1.749788e-02

# $lnLik
# [1] -1862.631

# $counts
# [1] 366

# $convergence
# [1] 0
```
• Define different constrain models

```r
# define constrain equal (q01 = q10)

starting_values_birds_migration[1:5]
migratory_constrain_transition_rate_BiSSE.lik <- constrain(birds_migration_BiSSE_full.lik, q01 ~ q10)
constratin_trasition_rate_BiSSE_mle <- find.mle
(migratory_constrain_trasition_rate_BiSSE.lik, starting_values_birds_migration[1:5])
constratin_trasition_rate_BiSSE_mle

# $par
# lambda0   lambda1       mu0      mu1      q01
# 3.941650e-02 5.175425e-02 7.375324e-07 1.484734e-02 8.733015e-03

# $lnLik
# [1] -1866.894

# $counts
# [1] 343

# $convergence
# [1] 0
```
• Make a list of coefficients for full and constrain BiSSE models

```r
install.packages("gtools")
library(gtools)

migration_full <- coef(birds_migration_BiSSE_full_mle)
speciation_cons <- coef(constratin_speciation_rate_BisSSE_mle)
transition_cons <- coef(constratin_trasition_rate_BisSSE_mle)

all_models <- smartbind(migration_full, speciation_cons, transition_cons)
rownames(all_models) <- c("full", "equal_lambda", "equal_transition")
all_models
```

```
#                     lambda0    lambda1          mu0          mu1         q01        q10
# full             0.03296855 0.05208791 0.000000e+00 0.0000000000 0.003888446 0.02504977
# equal_lambda     NA 0.04059865 3.272882e-05 0.0000089472 0.006441251 0.01749788
# equal_transition 0.03941650 0.05175425 7.375324e-07 0.0148473383 0.008733015  NA
```

Trait Evolution under BiSSE model in ‘diversitree’
## Trait Evolution under BiSSE model in ‘diversitree’

- Compare full and constrain BiSSE models

```r
anova(birds_migration_BiSSE_full_mle, equal_speciation =
constratin_speciation_rate_BiSSE_mle)

#      Df  lnLik  AIC  ChiSq Pr(>|Chi|)
# full  6 -1856.4 3724.9
# equal_speciation  5 -1862.6 3735.3 12.373 0.0004356 ***
# ***
# Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Rejects: equal speciation then lambda1 > lambda0 (migratory speciate more)
```

```r
anova(birds_migration_BiSSE_full_mle, equal_transition =
constratin_trasition_rate_BiSSE_mle)

#      Df  lnLik  AIC  ChiSq Pr(>|Chi|)
# full  6 -1856.4 3724.9
# equal_transition  5 -1866.9 3743.8 20.898 4.843e-06 ***
# ***
# Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Rejects: equal rates then q10 > q01 (higher rate of transition from migratory to non-migratory)
```
Trait Evolution under BiSSE model in ‘diversitree’

• Reconstruct and plot ancestral reconstructions for each node

```r
birds_migration_bisse_anc.states <- asr.marginal(birds_migration_BiSSE_full.lik, 
birds_migration_BiSSE_full_mle$par)
birds_migration_bisse_anc.states_t <- t(birds_migration_bisse_anc.states)
```

• Plot ancestral reconstructions for each node

```r
plot(birds_migration_phy, no.margin=TRUE, cex=0.5, label.offset=4, type = "fan")
tip_colors <- rep('blue', times=length(birds_migration_dat_bin)) # we are going to create a 
vector and consider blue -- no migratory

tip_colors[birds_migration_dat_bin == 1] <- 'red' # assign color red to migratory birds

tiplabels(bg=tip_colors, pch=21, adj=2.5) # Plot the tip labels on tree

nodeplabels(pie=birds_migration_bisse_anc.states_t, piecol=c("blue","red"), cex=0.12)
```
Trait Evolution under BiSSE model in ‘diversitree’

- Plot ancestral reconstructions for each node
Bayesian estimation of diversification and character transition rates in BiSSE

• We need our full BiSSE Model

```
birds_migration_BiSSE_full.lik <- make.bisse(birds_migration_phy, birds_migration_dat_bin) argnames(birds_migration_BiSSE_full.lik)
```

• We need our full BiSSE Model need starting values

```
starting_values_birds_migration <- starting.point.bisse(birds_migration_phy) starting_values_birds_migration

#   lambda0   lambda1     mu0     mu1     q01     q10
# 0.040574788 0.040574788 0.000000000 0.000000000 0.008114958 0.008114958
```

• From BiSSE tutorial: Because we are fitting six parameters to a tree, priors will be needed so that the posterior distribution is proper. I will use an exponential prior with rate 1/(2r), where r is the character independent diversification rate:

```
lambda0 - mu0 \rightarrow starting_values_birds_migration[1] - starting_values_birds_migration[3])
```

```
prior_bisse_birds <- make.prior.exponential(1 / (2 * (starting_values_birds_migration[1] - starting_values_birds_migration[3]))))
```
Bayesian estimation of diversification and character transition rates in BiSSE

• From BiSSE tutorial: First tuning of the MCMC sampler in diversitree uses slice sampling for parameter updates. **We then get the “step size” (argument \( w \)) does not need to be carefully tuned – just a number of function evaluations per update. Ideally it will be on the same order as the width of the “high probability region”. An easy way of setting this is to run a short chain (say, 100 steps) and use the range**

```r
set.seed(1)
tmp <- mcmc(birds_migration_BiSSE_full.lik,
            birds_migration_BiSSE_full_mle$par,  # the parameters of the mle estimation
            nsteps=100,
            prior=prior_bisse_birds,
            lower=0,
            w=rep(1, 6),
            print.every=0)

w <- diff(sapply(tmp[2:7], range))  #“step size” (argument \( w \))
w
# lambda0    lambda1     mu0      mu1       q01       q10
# [1,] 0.01467212 0.02673207 0.01645717 0.02766532 0.009465902 0.01652097
```
Bayesian estimation of diversification and character transition rates in BiSSE

- We run our MCMC analysis. This will take some time ideally nsteps > 10000

```r
birds_samples_bisse_mcmc <- mcmc(birds_migration_BiSSE_full.lik,  
    birds_migration_BiSSE_full_mle$par,  # the parameters of the mle estimation  
    nsteps=900,  
    prior=prior_bisse_birds,  # our prior  
    w=w,  # “step size” (argument w)  
    print.every=1000)
```

# 100: {0.0388, 0.0584, 0.0056, 0.0067, 0.0058, 0.0261} -> -1846.98262
# 200: {0.0335, 0.0584, 0.0022, 0.0053, 0.0032, 0.0297} -> -1845.93237
# 300: {0.0344, 0.0517, 0.0094, 0.0070, 0.0034, 0.0257} -> -1847.65817
# 400: {0.0389, 0.0599, 0.0152, 0.0041, 0.0034, 0.0384} -> -1851.45420
# 500: {0.0360, 0.0514, 0.0038, 0.0013, 0.0041, 0.0234} -> -1844.29190
# 600: {0.0322, 0.0581, 0.0019, 0.0089, 0.0047, 0.0224} -> -1845.16370
# 700: {0.0309, 0.0579, 0.0021, 0.0049, 0.0043, 0.0206} -> -1846.43910
# 800: {0.0395, 0.0619, 0.0075, 0.0076, 0.0036, 0.0248} -> -1847.61478
# 900: {0.0346, 0.0607, 0.0032, 0.0081, 0.0060, 0.0263} -> -1845.90865
Bayesian estimation of diversification and character transition rates in BiSSE

- We can review our results

```r
head(birds_samples_bisse_mcmc)
#  i  lambda0  lambda1  mu0  mu1   q01   q10    p
# 1  1  0.03645597  0.05072918  0.0035214865  0.004613237  0.02636477 -1844.197
# 2  2  0.03723505  0.05887234  0.0055874431  0.0048106318  0.005958448  0.03495245 -1848.445
# 3  3  0.03565244  0.05908928  0.0109415107  0.004911595  0.004911595  0.02709003 -1847.669
# 4  4  0.04431709  0.05631060  0.0083164813  0.0116621165  0.002523015  0.01818347 -1852.252
# 5  5  0.03164067  0.06295866  0.0020569494  0.0123037048  0.006906132  0.02633448 -1846.994
# 6  6  0.03320673  0.06361841  0.0005813076  0.0076708621  0.006601689  0.02706493 -1846.321

# get some estimates

install.packages("matrixStats")
library(matrixStats)

colMax <- function(data) sapply(data, max, na.rm = TRUE)
colMin <- function(data) sapply(data, min, na.rm = TRUE)

bissie_means <- colMeans(birds_samples_bisse_mcmc[(0.2 * 900):900,]) # we discard 20% of the initial data
bissie_sd <- colSds(as.matrix(birds_samples_bisse_mcmc[(0.2 * 900):900,]))
bissie_IQR <- colIQRs(as.matrix(birds_samples_bisse_mcmc[(0.2 * 900):900,]))
bissie_max <- colMax(birds_samples_bisse_mcmc[(0.2 * 900):900,])
bissie_min <- colMin(birds_samples_bisse_mcmc[(0.2 * 900):900,])
bissie_count <- rep(nrow(birds_samples_bisse_mcmc[(0.2 * 900):900,]), 8)
bissie_95CI <- 1.96*(bissie_sd/(bissie_count^0.5))
bissie_95CI_L <- bissie_means - bissie_95CI
bissie_95CI_U <- bissie_means + bissie_95CI
```
Bayesian estimation of diversification and character transition rates in BiSSE

- We can review our results

```r
bissie_stats <- rbind(bissie_means, bissie_sd, bissie_count, bissie_95CI_L, bissie_95CI_U, bissie_max, bissie_min)
bissie_stats <- bissie_stats[,-1]
bissie_stats
format(bissie_stats, scientific = FALSE, digits = 4)
bissie_stats
```

<table>
<thead>
<tr>
<th>lambda0</th>
<th>lambda1</th>
<th>mu0</th>
<th>mu1</th>
<th>q0</th>
<th>q1</th>
<th>p</th>
</tr>
</thead>
<tbody>
<tr>
<td>bissie_means</td>
<td>3.449583e-02</td>
<td>5.634769e-02</td>
<td>3.693126e-03</td>
<td>6.230848e-03</td>
<td>4.601787e-03</td>
<td>2.596785e-02</td>
</tr>
<tr>
<td>bissie_sd</td>
<td>3.146553e-03</td>
<td>5.638784e-03</td>
<td>3.520198e-03</td>
<td>5.625421e-03</td>
<td>1.617453e-03</td>
<td>4.497347e-03</td>
</tr>
<tr>
<td>bissie_count</td>
<td>7.210000e+02</td>
<td>7.210000e+02</td>
<td>7.210000e+02</td>
<td>7.210000e+02</td>
<td>7.210000e+02</td>
<td>7.210000e+02</td>
</tr>
<tr>
<td>bissie_95CI_L</td>
<td>3.426615e-02</td>
<td>5.593609e-02</td>
<td>3.436172e-03</td>
<td>5.820224e-03</td>
<td>4.483723e-03</td>
<td>2.563957e-02</td>
</tr>
<tr>
<td>bissie_95CI_U</td>
<td>3.472551e-02</td>
<td>5.675929e-02</td>
<td>3.950080e-03</td>
<td>6.641471e-03</td>
<td>4.719852e-03</td>
<td>2.629613e-02</td>
</tr>
<tr>
<td>bissie_max</td>
<td>4.389477e-02</td>
<td>7.942649e-02</td>
<td>2.031885e-02</td>
<td>3.297781e-02</td>
<td>1.015513e-02</td>
<td>3.997918e-02</td>
</tr>
<tr>
<td>bissie_min</td>
<td>2.504994e-02</td>
<td>4.127147e-02</td>
<td>1.643737e-05</td>
<td>6.105504e-06</td>
<td>1.479920e-03</td>
<td>1.081088e-02</td>
</tr>
</tbody>
</table>
```
Finally plot our results

```r
col <- c("#004165", "#eaab00")
profiles.plot(birds_samples_bisse_mcmc[c("lambda0", "lambda1")], col.line=col, las=1, xlab="Speciation rate", legend="topright")
abline(v=c(.1, .2), col=col)

col <- c("purple", "blue")
profiles.plot(birds_samples_bisse_mcmc[c("mu0", "mul")], col.line=col, las=1, xlab="Speciation rate", legend="topright")
abline(v=c(.1, .2), col=col)

col <- c("green", "gray")
profiles.plot(birds_samples_bisse_mcmc[c("q01", "q10")], col.line=col, las=1, xlab="Speciation rate", legend="topright")
abline(v=c(.1, .2), col=col)
```
Bayesian estimation of diversification and character transition rates in BiSSE

- Finally plot our results
Multiple state characters and diversification: MuSSE

- It is useful for discrete character with more than two states

- The characters are coded as a matrix of multiple binary characters (0 -- absent, 1 -- present)

<table>
<thead>
<tr>
<th></th>
<th>Carnivore</th>
<th>Omnivore</th>
<th>Vegetarian</th>
</tr>
</thead>
<tbody>
<tr>
<td>SpA</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>SPB</td>
<td>0</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>SPC</td>
<td>0</td>
<td>0</td>
<td>1</td>
</tr>
</tbody>
</table>

- However, the coding of the states get very complex

\[ \lambda_0, \lambda_1, \lambda_2 \]
\[ \mu_0, \mu_1, \mu_2 \]
\[ q_{12}, q_{21}, q_{13} \]
\[ q_{31}, q_{23}, q_{32} \]

- More parameters means more likelihood space to explore and the issue of power has not been addressed
Other methods in ‘diversitree’

Quantitative traits and diversification: QuaSSE

• Most phenotypic traits are continuous (e.g., body mass, metabolic rates)
• Much more complicated analyses and very slow
• Uses a system of partial differential equations that relates the character values to diversification rates
• Issues of power and/or the accuracy of the estimators are unknown

Others:

Geographic distributions and diversification: GeoSSE

Cladogenetic State change Speciation and Extinction: ClaSSE

Binary-State Speciation and Extinction–node enhanced state shift: BiSSE-ness
Issues with the analysis using BiSSE

• Low power:

From Davies et al. (2013): Based on our findings, we recommend that future studies utilizing BiSSE that have fewer than 300 terminals and/or have datasets where high tip ratio bias is observed (i.e., fewer than 10% of species are of one character state) should be extremely cautious with the interpretation of hypothesis testing results

Davis et al. BMC Evolutionary Biology 2013, 13:38
http://www.biomedcentral.com/1471-2148/13/38

• We need large phylogenies, with low rate heterogeneity, and >10% of the species showing alternate states