Phylogenetic Inference using RevBayes

Historical biogeography

Michael J. Landis

Introduction

Many fundamental evolutionary processes, such as adaptation, speciation, and extinction, operate in a spatial context. When the historical aspect of this spatial context cannot be observed directly, as is often the case, biogeographic inference may be applied to estimate ancestral species ranges. This works by leveraging phylogenetic, molecular, and geographical information to model species distributions as the outcome of biogeographic processes. How to best model these processes requires special consideration, such as how ranges are inherited following speciation events, how geological events might influence dispersal rates, and what factors affect rates of dispersal and extirpation. A major technical challenge of modeling range evolution is how to translate these natural processes into stochastic processes that remain tractable for inference. This tutorial provides a brief background in some of these models, then describes how to perform Bayesian inference of historical biogeography using `RevBayes`.

Contents

The Historical Biogeography guide contains several tutorials

Recommended tutorials

The Historical Biogeography tutorials assume the reader is familiar with the content covered in the following `RevBayes` tutorials

- **`Rev` Basics**
- **Molecular Models of Character Evolution**
- **Running and Diagnosing an MCMC Analysis**
- **Divergence Time Estimation and Node Calibrations**

1 Overview of the Dispersal-Extinction-Cladogenesis model

The Dispersal-Extinction-Cladogenesis (DEC) process models range evolution as a discrete-valued process (Ree et al. 2005; Ree and Smith 2008). There are three key components to understanding the DEC model: range characters, anagenetic range evolution, and cladogenetic range evolution (Figure 1).

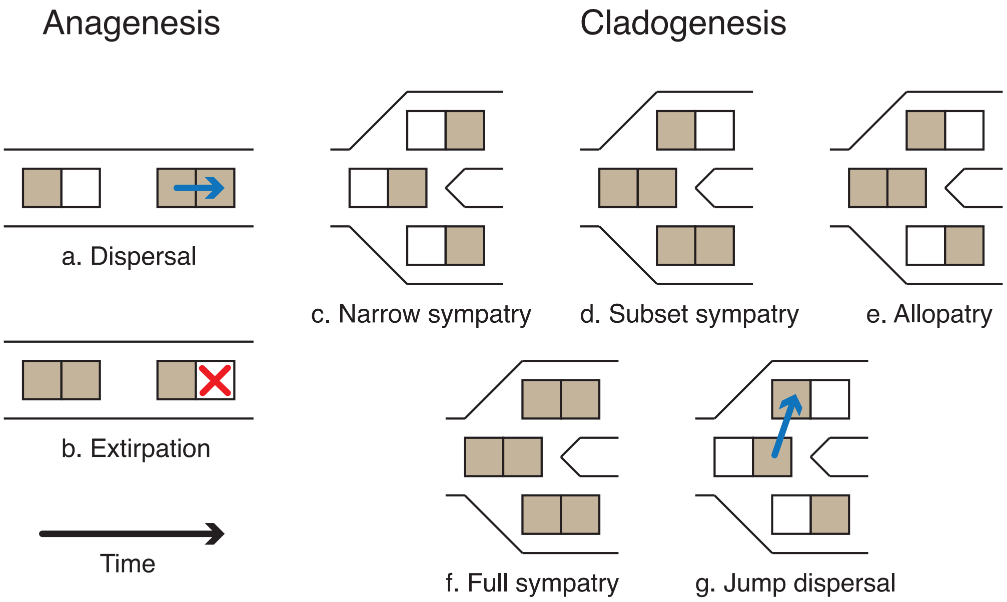


Figure 1: Cartoon of behavior of the DEC model. Two anagenetic events (a,b) and five cladogenetic (c–g) events are shown for a system with two areas. Areas are shaded when inhabited by a given lineage and left blank when uninhabited. Time proceeds from left to right. (a) Dispersal: a new area to be added to the species range. (b) Extirpation (or local extinction): the species range loses a previously inhabited area. (c) Narrow sympatry: When the ancestral range contains one area, both daughter lineages inherit that area. (d) Subset sympatry: When the ancestral range is widespread, one daughter inherits the ancestral range and the other daughter inherits only one area. (e) Allopatry (or vicariance): When the ancestral range is widespread, one daughter lineage a subset of the ancestral areas while the other daughter inherits all remaining ancestral areas. (f) Widespread sympatry: When the ancestral range is widespread, both daughters inherit the ancestral range. (g) Jump dispersal (or founder speciation): One daughter inherits the ancestral range while the other daughter inherits a new unoccupied area.

1.1 Discrete range characters

DEC interprets taxon ranges as presence-absence data, that is, where a species is observed or not observed across multiple discrete areas. For example, say there are three areas, A, B, and C. If a species is present in areas A and C, then its range equals AC, which can also be encoded into the length-3 bit vector, 101. Bit vectors may also be transformed into (decimal) integers, *e.g.,* the binary number 101 equals the decimal number 5.

The decimal representation of range states is rarely used in discussion, but it is useful to keep in mind when considering the total number of possible ranges for a species and when processing output.

Range	Bits	Size	State
∅	000	0	0
A	100	1	1
B	010	1	2
C	001	1	3
AB	110	2	4
AC	101	2	5
BC	011	2	6
ABC	111	3	7

Table 1: Example of discrete range representations for an analysis with areas A, B, and C.

1.2 Anagenetic range evolution

In the context of the DEC model, anagenesis refers to range evolution that occurs between speciation events within lineages. There are two types of anagenetic events, dispersal (Figure 1a) and (local) extinction or exitrpation (Figure 1b). Because DEC uses discrete-valued ranges, anagenesis is modeled using a continuous-time Markov chain. This, in turn, allows us to compute transition probability of a character changing from i to j in time t through matrix exponentiation

$$\mathbf{P}_{ij}(t) = \left[\exp\left\{\mathbf{Q}t\right\}\right]_{ij},$$

where $\mathbf{Q}$ is the instantaneous rate matrix defining the rates of change between all pairs of characters, and $\mathbf{P}$ is the transition probability rate matrix. The indices i and j represent different ranges, each of which is encoded as the set of areas occupied by the species. The probability has integrated over all possible scenarios of character transitions that could occur during t so long as the chain begins in range i and ends in range j. We can then encode $\mathbf{Q}$ to reflect the allowable classes of range evolution events with biologically meaningful parameters. For three areas, the rates in the anagenetic rate matrix are

$$\mathbf{Q} = \begin{array}{c|cccccccc}
 & \emptyset & A & B & C & AB & AC & BC & ABC \\
\hline
\emptyset & - & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
A & e_A & - & 0 & 0 & d_{AB} & d_{AC} & 0 & 0 \\
B & e_B & 0 & - & 0 & d_{BA} & 0 & d_{BC} & 0 \\
C & e_C & 0 & 0 & - & 0 & d_{CA} & d_{CB} & 0 \\
AB & 0 & e_A & e_B & 0 & - & 0 & 0 & d_{AC}+d_{BC} \\
AC & 0 & e_C & 0 & e_A & 0 & - & 0 & d_{AB}+d_{CB} \\
BC & 0 & 0 & e_C & e_B & 0 & 0 & - & d_{BA}+d_{CA} \\
ABC & 0 & 0 & 0 & 0 & e_C & e_B & e_A & -
\end{array}$$

where $e = (e_A, e_B, e_C)$ are the (local) extinction rates per area, and $d = (d_{AB}, d_{AC}, d_{BC}, d_{BA}, d_{CA}, d_{CB})$ are the dispersal rates between areas. Notice that the sum of rates leaving the null range ($\emptyset$) is zero, meaning any lineage that loses all areas in its range remains that way permanently.

To build our intuition, let's construct a DEC rate matrix in `RevBayes`. Assume you have three areas

```
n_areas <- 3
```

First, create a matrix of dispersal rates between area pairs, with rates $d_{AB} = d_{AC} = \ldots = d_{CB} = 1$.

```
for (i in 1:n_areas) {
    for (j in 1:n_areas) {
        dr[i][j] <- 1.0
    }
}
```

Next, let's create the extirpation rates with values $e_A = e_B = e_C = 1$

```
for (i in 1:n_areas) {
    for (j in 1:n_areas) {
        er[i][j] <- 0.0
    }
    er[i][i] <- 1.0
}
```

When the extirpation rate matrix is a diagonal matrix (i.e. all non-diagonal entries are zero), extirpation rates are mutually independent as in (Ree et al. 2005). More complex models that penalize widespread ranges that span disconnected areas are explored in later sections.

To continue, create the DEC rate matrix from the dispersal rates (`dr`) and extirpation rates (`er`).

```
Q_DEC := fnDECRateMatrix(dispersalRates=dr, extirpationRates=er)
Q_DEC
[ [ 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000 ] ,
    1.0000, -3.0000, 0.0000, 0.0000, 1.0000, 1.0000, 0.0000, 0.0000 ] ,
    1.0000, 0.0000, -3.0000, 0.0000, 1.0000, 0.0000, 1.0000, 0.0000 ] ,
    1.0000, 0.0000, 0.0000, -3.0000, 0.0000, 1.0000, 1.0000, 0.0000 ] ,
    0.0000, 1.0000, 1.0000, 0.0000, -4.0000, 0.0000, 0.0000, 2.0000 ] ,
    0.0000, 1.0000, 0.0000, 1.0000, 0.0000, -4.0000, 0.0000, 2.0000 ] ,
    0.0000, 0.0000, 1.0000, 1.0000, 0.0000, 0.0000, -4.0000, 2.0000 ] ,
    0.0000, 0.0000, 0.0000, 0.0000, 1.0000, 1.0000, 1.0000, -3.0000 ] ]
```

Compute the anagenetic transition probabilities for a branch of length `0.2`.

```
tp_DEC <- Q_DEC.getTransitionProbabilities(rate=0.2)
tp_DEC
[ [ 1.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000],
  [ 0.000, 0.673, 0.013, 0.013, 0.123, 0.123, 0.005, 0.050],
  [ 0.000, 0.013, 0.673, 0.013, 0.123, 0.005, 0.123, 0.050],
  [ 0.000, 0.013, 0.013, 0.673, 0.005, 0.123, 0.123, 0.050],
  [ 0.000, 0.107, 0.107, 0.004, 0.502, 0.031, 0.031, 0.218],
  [ 0.000, 0.107, 0.004, 0.107, 0.031, 0.502, 0.031, 0.218],
  [ 0.000, 0.004, 0.107, 0.107, 0.031, 0.031, 0.502, 0.218],
  [ 0.000, 0.021, 0.021, 0.021, 0.107, 0.107, 0.107, 0.616]]
```

Notice how the structure of the rate matrix is reflected in the transition probability matrix. For example, ranges that are separated by multiple dispersal and extirpation events are the most improbable: transitioning from going from A to BC takes a minimum of three events and has probability 0.005.

Also note that the probability of entering or leaving the null range is zero. By default, the `RevBayes` conditions the anagenetic range evolution process on never entering the null range when computing the transition probabilities (`nullRange="CondSurv"`). This allows the model to both simulate and infer using the same transition probabilities. Massana et al. (2015) first noted that the null range—an unobserved absorbing state—results in abnormal extirpation rate and range size estimates. Their proposed solution to eliminate the null range from the state space is enabled with the `nullRange="Exclude"` setting. The `nullRange="Include"` setting provides no special handling of the null range, and produces the raw probabilities of Ree et al. (2005).

1.3 Cladogenetic range evolution

The cladogenetic component of the DEC model describes evolutionary change accompanying speciation events (Figure 1c–g). In the context of range evolution, daughter species do not necessarily inherit their ancestral range in an identical manner. For each internal node in the reconstructed tree, one of several cladogenetic events can occur, some of which are described below.

Beginning with the simplest case first, suppose the range of a species is A the moment before speciation occurs at an internal phylogenetic node. Since the species range is size one, both daughter lineages necessarily inherit the ancestral species range (A). In DEC parlance, this is called a narrow sympatry event (Figure 1c). Now, suppose the ancestral range is ABC. Under subset sympatry, one lineage identically inherits the ancestral species range, ABC, while the other lineage inherits only a single area, i.e. only A or B or C (Figure 1d). Under allopatric cladogenesis, the ancestral range is split evenly among daughter lineages, e.g. one lineage may inherit AB and the other inherits C (Figure 1e). For widespread sympatric cladogenesis, both lineages inherit the ancestral range, ABC (Figure 1f). Finally, supposing the ancestral range is A, jump dispersal cladogenesis results in one daughter lineage inheriting the ancestral range A, and the other daughter lineage inheriting a previously uninhabited area, B or C (Figure 1g). See Matzke (2012) for an excellent overview of the cladogenetic state transitions described in the literature.

Make the cladogenetic probability event matrix

```
clado_event_types = [ "s", "a" ]
clado_event_probs <- simplex( 1, 1 )
P_DEC := fnDECCladoProbs(eventProbs=clado_event_probs,
                         eventTypes=clado_event_types,
                         numCharacters=n_areas)
```

`clado_event_types` defines what cladogenetic event types are used. `"a"` and `"s"` indicate allopatry and subset sympatry, as described in (Ree et al. 2005). Other cladogenetic events include jump dispersal (`"j"`;

?) and full sympatry (`"f"`; Landis et al. 2013). The cladogenetic event probability matrix will assume that `eventProbs` and `eventTypes` share the same order.

Print the cladogenetic transition probabilities

```
P_DEC
   [
     ( 1 -> 1, 1 ) = 1.0000,
     ( 2 -> 2, 2 ) = 1.0000,
     ( 3 -> 3, 3 ) = 1.0000,
     ...
     ( 7 -> 7, 1 ) = 0.0833,
     ( 7 -> 7, 2 ) = 0.0833,
     ( 7 -> 7, 3 ) = 0.0833
   ]
```

The cladogenetic probability matrix becomes very sparse for large numbers of areas, so only non-zero values are shown. Each row reports a triplet of states—the ancestral state and the two daughter states—with the probability associated with that event. Since these are proper probabilities, the sum of probabilities for a given ancestral state over all possible cladogenetic outcomes equals one.

1.4 Things to consider

The probabilities of anagenetic change along lineages must account for all combinations of starting states and ending states. For 3 areas, there are 8 states, and thus $8 \times 8 = 64$ probability terms for pairs of states. For cladogenetic change, we need transition probabilities for all combinations of states before cladogenesis, after cladogenesis for the left lineage, and after cladogenesis for the right lineage. Like above, for three areas, there are 8 states, and $8 \times 8 \times 8 = 512$ cladogenetic probability terms.

Of course, this model can be specified for more than three areas. Let's consider what happens to the size of $\mathbf{Q}$ when the number of areas, N, becomes large. For three areas, $\mathbf{Q}$ is size 8×8. For ten areas, $\mathbf{Q}$ is size $2^{10} \times 2^{10} = 1024 \times 1024$, which approaches the largest size matrices that can be exponentiated in a practical amount of time. For twenty areas, $\mathbf{Q}$ is size $2^{20} \times 2^{20} \approx 10^6 \times 10^6$ and exponentiation is not viable. Thus, selecting the discrete areas for a DEC analysis should be done with regard to what one hopes to learn through the analysis itself.

1.5 Some questions

$\boxed{?}$ **For the three-area DEC rate matrix above, what is the rate of leaving state AC in terms of dispersal and extinction parameters?**

$\boxed{?}$ **What series of transition events might explain a lineage evolving from range ABC to range A? From range AB to range C? (Hint: more than one event is needed!)**

$\boxed{?}$ **Imagine a DEC rate matrix with four areas, $ABCD$. What would be the dispersal rate for $Q_{BC,BCD}$? How many states does a DEC rate matrix with four areas have? What is the relationship between the number of areas and the number of states under the DEC model?**

$\boxed{?}$ **Given the state is** AB **before cladogenesis, and allowing subset sympatry, widespread sympatry, and allopatry, what are the 7 possible states in the daughter lineages after cladogenesis?**

$\boxed{?}$ **For three areas, there are three narrow, four widespread, 18 subset sympatric events, and 12 allopatric cladogenesis events. What proportion of terms in the cladogenesis matrix are zero?**

2 Simple DEC analysis

The following series of tutorials will estimate the ancestral ranges of the silversword alliance (Tribe *Madiinae*), a young and diverse clade of about 50 species and subspecies. Although silverswords are endemic to Hawaii, they are nested within a larger clade alongside tarweeds, which are native to western continental North America (Baldwin et al. 1991). The size and age of the silversword clade, combined with our knowledge of Hawaiian island formation, makes it an ideal system to explore concepts in historical biogeography and phylogeny. For further reading, consult: Carlquist (1959); Baldwin and Sanderson (1998).

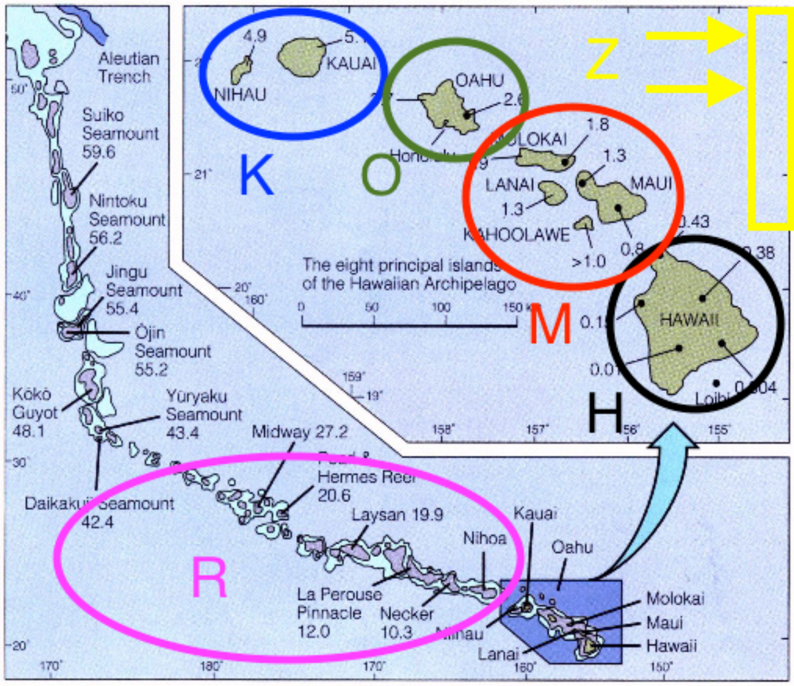


Figure 2: A beautiful figure of the discrete areas for the tutorial. Six areas are shown: Kauai and Niihau (K); Oahu (O); Maui-Nui, Lanai, and Molokai (M); Hawaii (H); the remaining Hawaiian islands (R); and the North American mainland (Z).

For this tutorial we'll focus entirely on the silversword alliance and the modern Hawaiian archipelago. To begin, we'll use just four areas, K, O, M, and H, and include areas R and Z in later analyses (Figure 2). The species ranges used in this exercise follow Gillespie and Baldwin (2009).

Analysis

First, create file management variables for input and output

```
range_fn = "data/n4/silversword.n4.range.nex"
tree_fn = "data/n4/silversword.tre"
out_fn = "output/simple"
```

then read in our character data as binary presence-absence characters

Range	Areas	Size	State
∅	0000	0	0
K	1000	1	1
O	0100	1	2
M	0010	1	3
H	0001	1	4
KO	1100	2	5
KM	1010	2	6
OM	0110	2	7
KH	1001	2	8
OH	0101	2	9
MH	0011	2	10
KOM	1110	3	11
KOH	1101	3	12
KMH	1011	3	13
OMH	0111	3	14
KOMH	1111	4	15

Table 2: Area coding used for four areas: K is Kauai and Nihoa; O is Oahu; M is Maui Nui, Lanai, and Molokai; H is Hawaii island.

```
dat_range_01 = readDiscreteCharacterData(range_fn)
```

then encode the species ranges into natural numbers

```
dat_range_n   = formatDiscreteCharacterData(dat_range_01, "DEC")
```

Record the number of areas (characters) from the discrete character data object

```
n_areas = dat_range_01.nchar()
```

You can view the taxon data to see how characters are coded both as human-readable presence-absence data and as computer-readable natural numbers

```
dat_range_01[1]
  Argyroxiphium_grayanum_East_Maui:
    0010
dat_range_n[1]
  Argyroxiphium_grayanum_East_Maui:
    3
```

We'll want to record the relationship between range states and range labels when producing an ancestral range estimate figure. First, store the vector of range state descriptions

```
state_desc = dat_range_n.getStateDescriptions()
```

then write it to file

```
state_desc_str = "state,range\n"
for (i in 1:state_desc.size())
{
    state_desc_str += (i-1) + "," + state_desc[i] + "\n"
}
write(state_desc_str, file=out_fn+".state_labels.txt")
```

For this tutorial we'll assume we know the dated species phylogeny without error.

```
tree <- readTrees(tree_fn)[1]
```

Next, we'll build the anagenetic rate matrix for the DEC model. In its simplest form, the rate matrix requires a dispersal rate and an extirpation rate. For this analysis, we'll assume that all pairs of areas share the same dispersal rate and all areas share the same extirpation rate. To gain greater control to observe and manage prior sensitivity, we'll reparameterize the DEC rate matrix to report the *relative* rates of dispersal versus extirpation events. In order for anagenetic event rates to be measured on an absolute time scale (e.g. in millions of years), we will also introduce a a biogeographic rate parameter, similar to the molecular clock parameter used in dating analyses.

First, create a parameter for the arrival rate of anagenetic range evolution events. We'll apply an uninformative prior to the rate's magnitude by first assigning a uniform distribution to the $\log_{10}$ rate.

```
log10_rate_bg ~ dnUniform(-4,2)
log10_rate_bg.setValue(-2)
moves[1] = mvSlide(log10_rate_bg, weight=4)
```

then convert the rate from log-scale to linear-scale with a deterministic node

```
rate_bg := 10^log10_rate_bg
```

This yields a uniform prior over orders of magnitude, ranging from 10^{-4} to 10^{2} events per million years.

Because the rate matrix will describe the relative anagenetic event rates, we can safely assume that dispersal occurs at the relative (fixed) rate of one.

```
dispersal_rate <- 1.0
```

then create the dispersal rate matrix

```
for (i in 1:n_areas) {
  for (j in 1:n_areas) {
    dr[i][j] <- dispersal_rate
  }
}
```

Next, assign a prior distribution to the relative extirpation rate and assign it a move. The prior distribution of extirpation rates is given `log_sd` and `log_mean` values that give the prior expected value of one – i.e. the mean rate of area gain and area loss are equal under the prior.

```
log_sd <- 0.5
log_mean <- ln(1) - 0.5*log_sd^2
extirpation_rate ~ dnLognormal(mean=log_mean, sd=log_sd)
moves[2] = mvScale(extirpation_rate, weight=2)
```

then create a matrix of extirpation rates

```
for (i in 1:n_areas) {
  for (j in 1:n_areas) {
    er[i][j] <- 0.0
  }
  er[i][i] := extirpation_rate
}
```

Note that `er` is a diagonal matrix whose diagonal values are determined (`:=`) by the stochastic variable, `extirpation_rate`. We can now create our relative rate matrix, `Q_DEC`, with the `fnDECRateMatrix` function.

```
Q_DEC := fnDECRateMatrix(dispersalRates=dr, extirpationRates=er)
```

Note, `fnDECRateMatrix` does not rescale its elements in any way, so transition rates share the same time scale as the underlying tree. This scaling is in contrast to the standard molecular substitution processes that are available in `RevBayes`, such as `fnGTR`, whose rates are rescaled such that the process is expected to produce one event per site per unit time.

Next, we need to create the cladogenetic probability matrix. Cladogenetic event probabilities are given by a transition probability matrix, not a rate matrix. First, we will provide the vector `[ "s", "a" ]` to indicate that we wish to consider only subset sympatry and allopatry events. Next, we will create a vector of prior weights on cladogenesis events that fixes all cladogenetic events to be equiprobable.

```
clado_event_types <- [ "s", "a" ]
clado_event_probs <- simplex(1, 1)
P_DEC := fnDECCladoProbs(eventProbs=clado_event_probs,
                         eventTypes=clado_event_types,
                         numCharacters=n_areas)
```

Finally, all our DEC model components are encapsulated in the `dnPhyloCTMCClado` distribution, which is similar to `dnPhyloCTMC` except specialized to integrate over cladogenetic events. Although this dataset has four areas, it is recognized single character with states valued from 1 to 2^4, hence `nSites=1`.

```
m_bg ~ dnPhyloCTMCClado(tree=tree,
                        Q=Q_DEC,
                        cladoProbs=P_DEC,
                        branchRates=rate_bg,
                        nSites=1,
                        type="NaturalNumbers")
```

Finally, attach the observed ranges to the model. Be sure to use the natural number valued range characters, `dat_range_n`, and not the presence-absence range characters, `dat_range_01`.

```
m_bg.clamp(dat_range_n)
```

Add the monitors.

```
monitors[1] = mnScreen(rate_bg, extirpation_rate, printgen=100)
monitors[2] = mnModel(file=out_fn+".params.log", printgen=10)
monitors[3] = mnFile(tree, file=out_fn+".tre", printgen=10)
monitors[4] = mnJointConditionalAncestralState(tree=tree,
                                               ctmc=m_bg,
                                               filename=out_fn+".states.log",
                                               type="NaturalNumbers",
                                               printgen=10,
                                               withTips=true,
                                               withStartStates=true)
```

The `mnJointConditionalAncestralState` monitor samples ancestral states from the phylogeny, `tree`, according to the model of evolution, `m_bg`, and stores it to the file named `"simple.states.log"`. Each row in the states file lists the joint sample of ancestral states conditioned on the tip values for the entire tree (i.e. a *joint* ancestral state sample *conditional* on the tip states). Each column corresponds to the phylogenetic node index for that particular MCMC sample. The index is used used to match the state samples with the tree samples, which is especially important when the topology is a random variable (Section 4).

The remaining tasks should be familiar from previous tutorials, so we can proceed briskly. Prepare the model graph for analysis by creating a `Model` object.

```
mymodel = model(m_bg)
```

Create the `MCMC` object from the model, moves, and monitors variables, and run the MCMC analysis.

```
mymcmc = mcmc(mymodel, moves, monitors)
mymcmc.run(3000)
```

Results

Example results are located at `output_example/simple.*`

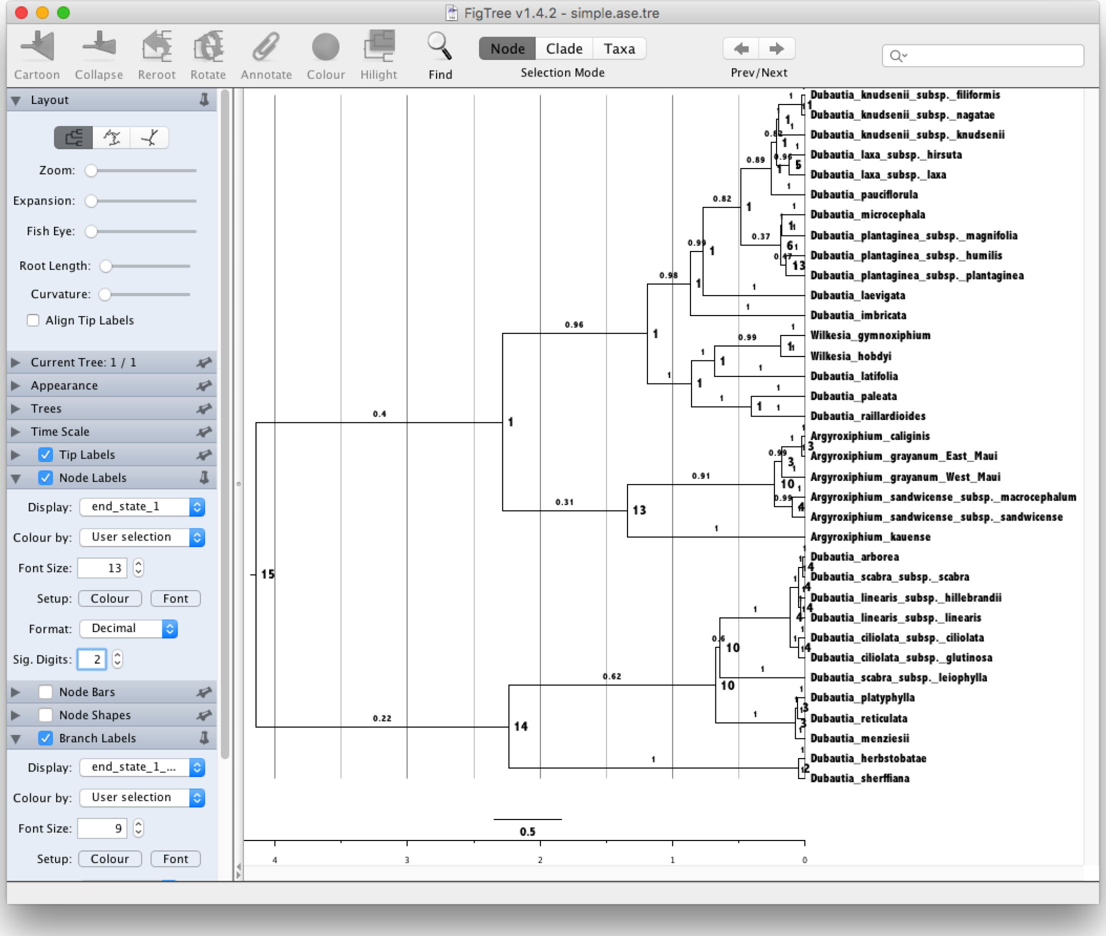
The script located at `scripts/make_anc_states.Rev` contains code to construct an ancestral state tree. Like all `RevBayes` scripts, this script may be executed from the command line. Because this is the first time using the script, we'll enter the code manually. To use it for future analyses, just modify the `out_str` variable to match the prefix of the target analysis, save the file, then execute the script by typing `"rb scripts/make_anc_states.Rev"` into the command line.

After opening a new `RevBayes` session, create helper variables for files we'll work with.

```
out_str = "output/simple"
out_state_fn = out_str + ".states.log"
out_tree_fn = out_str + ".tre"
out_mcc_fn = out_str + ".mcc.tre"
```

Build a maximum clade credibility tree from the posterior tree distribution, discarding the first 25% of samples. (Note, this step is gratuitous when we assume a fixed phylogeny, but essential when we estimate the phylogeny in Section 4).

```
tree_trace = readTreeTrace(file=out_tree_fn, treetype="clock")
tree_trace.setBurnin(0.25)
n_burn = tree_trace.getBurnin()
```


FigTree v1.4.2 - simple.ase.tre
Cartoon
Collapse
Reroot
Rotate
Annotate
Colour
Hilight
Find
Node
Clade
Taxa
Selection Mode
Prev/Next
Layout
Zoom:
Expansion:
Fish Eye:
Root Length:
Curvature:
Align Tip Labels
Current Tree: 1 / 1
Appearance
Trees
Time Scale
Tip Labels
Node Labels
Node Bars
Node Shapes
Branch Labels
Dubautia_knudsenii_subsp._filiformis
Dubautia_knudsenii_subsp._nagatae
Dubautia_knudsenii_subsp._knudsenii
Dubautia_laxa_subsp._hirsuta
Dubautia_laxa_subsp._laxa
Dubautia_pauciflorula
Dubautia_microcephala
Dubautia_plantaginea_subsp._magnifolia
Dubautia_plantaginea_subsp._humilis
Dubautia_plantaginea_subsp._plantaginea
Dubautia_laevigata
Dubautia_imbricata
Wilkesia_gymnoxiphium
Wilkesia_hobdyi
Dubautia_latifolia
Dubautia_paleata
Dubautia_raillardioides
Argyroxiphium_caliginis
Argyroxiphium_grayanum_East_Maui
Argyroxiphium_grayanum_West_Maui
Argyroxiphium_sandwicense_subsp._macrocephalum
Argyroxiphium_sandwicense_subsp._sandwicense
Argyroxiphium_kauense
Dubautia_arborea
Dubautia_scabra_subsp._scabra
Dubautia_linearis_subsp._hillebrandii
Dubautia_linearis_subsp._linearis
Dubautia_ciliolata_subsp._ciliolata
Dubautia_ciliolata_subsp._glutinosa
Dubautia_scabra_subsp._leiophylla
Dubautia_platyphylla
Dubautia_reticulata
Dubautia_menziesii
Dubautia_herbstobatae
Dubautia_sherffiana
15
14
13
10
0.4
0.22
0.31
0.96
0.62
0.98
0.91
0.5
4
3
2
1
0

Node Labels: Display: end_state_1; Colour by: User selection; Font Size: 13; Setup: Colour, Font; Format: Decimal; Sig. Digits: 2

Branch Labels: Display: end_state_1_...; Colour by: User selection; Font Size: 9; Setup: Colour, Font

Figure 3: Annotated tree with ancestral state estimates in FigTree. This tree was generated by ancestralStateTree in RevBayes. The most probable end state of each branch (before cladogenesis) is shown at each node. Branches are labeled with the posterior probability for the ancestral state on the tipwards end of the branch.

Compute and save the maximum clade credibility tree

```
mcc_tree = mccTree(tree_trace, file=out_mcc_fn)
```

Get the ancestral state trace from `simple.states.log`

```
state_trace = readAncestralStateTrace(file=out_state_fn)
```

Get the ancestral state tree trace from `simple.tre`. It is important to use `readAncestralTreeTrace` and not `readTreeTrace` to properly annotate the tree with ancestral states.

```
tree_trace = readAncestralStateTreeTrace(file=out_tree_fn, treetype="clock")
```

Finally, compute and save the ancestral state tree as `simple.ase.tre`.

```
anc_tree = ancestralStateTree(tree=mcc_tree,
                           ancestral_state_trace_vector=state_trace,
                           tree_trace=tree_trace,
                           include_start_states=true,
                           file=out_str+".ase.tre",
                           burnin=n_burn,
                           site=0)
```

We can review the output from `ancestralStateTree` in `FigTree` (Figure 3).

Ancestral state trees are annotated with the first three most probable ancestral states along with their posterior probabilities. When the tree is a random variable, as it is in later exercises, additional information about phylogenetic uncertainty is reported.

Finally, we can also generate a figure with ancestral states that is suitable for publication using the `R` package `RevGadgets` (Figure 4). The script is easily modified for use with different datasets. To create build a figure, open an `R` session and load the plotting script with the `source` function

```
source("plot_anc_state.simple.R")
```

Notice that the model infers a widespread ancestral range for the clade (KOMH) approximately four million years ago when only Kauai existed. Similar geologically unrealistic widespread ranges are estimated for the *Agyroxiphium* clade (KMH) and the *D. sheriffiana* and *D. arborea* clade (OMH). The remaining tutorials will focus on improvements to the simple DEC model presented here.

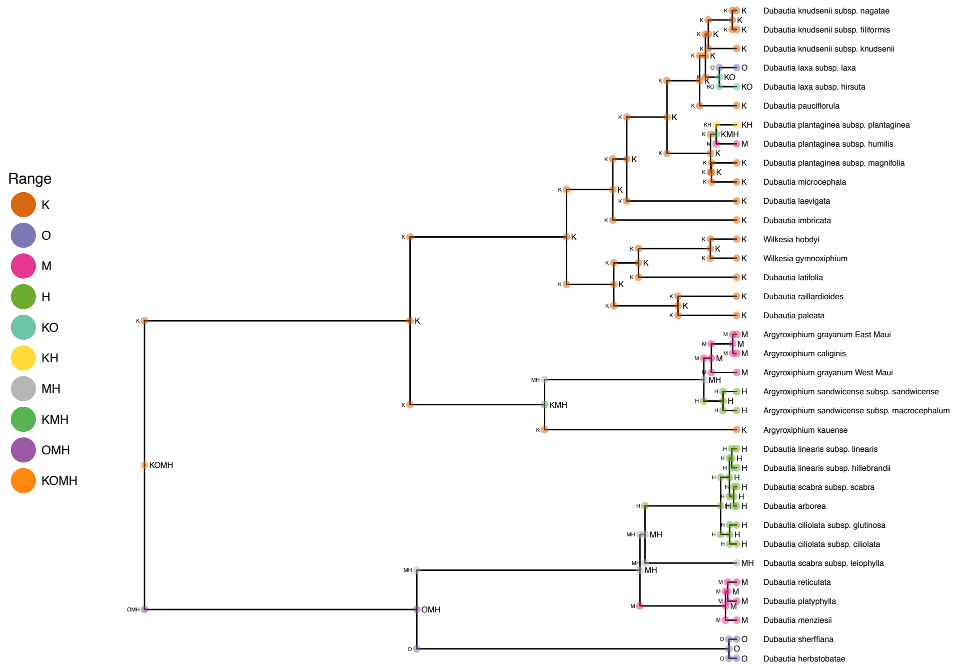


Figure 4: Tree with ancestral state estimates for the "simple" analysis. Nodes are annotated with ancestral states before and after cladogenetic events. The ancestral range with the highest posterior probability is shown. Colors of markers indicate the range state.

3 An improved DEC analysis

In this section, we'll introduce a suite of model features that lend towards more realistic biogeographic analyses. Topics include applying range size constraints, stratified (or epoch) models of paleoconnectivity, function-valued dispersal rates, and incorporating uncertainty in paleogeographic event time estimates. These modifications should produce more realistic ancestral range estimates, e.g. that a volcanic island may only be colonized once it has formed, and that distance should have some bearing on dispersal rate.

To accomplish this, we'll incorporate (paleo-)geographical data for the Hawaiian archipelago, summarized in Table 3. Even though we will continue to use four areas (K, O, M, H) in this section, we will use all six areas (R, K, O, M, H, Z) in Section 4, hence the full table is given for future reference.

3.1 Analysis

Start by creating variables for the tree file, the range data, and the output prefix

```
range_fn = "data/n4/silversword.n4.range.nex"
tree_fn = "data/n4/silversword.tre"
out_fn = "output/epoch"
```

area	code	a_{max}	a_{min}	$g_{\bullet R}$	$g_{\bullet K}$	$g_{\bullet O}$	$g_{\bullet M}$	$g_{\bullet H}$	$g_{\bullet Z}$
Older islands	R	-	-	-	261	406	500	680	3900
Kauai	K	5.15	5.05	-	-	145	239	419	3900
Oahu	O	3.7	2.2	-	-	-	059	239	3900
Maui Nui	M	1.8	1.3	-	-	-	-	082	3900
Hawaii	H	0.7	0.3	-	-	-	-	-	3900
Mainland	Z	-	-	-	-	-	-	-	-

Table 3: Hawaiian paleogeographic data. The six areas are given in Figure 2. Ages a_{max} and a_{min} report the maximum and minimum origination times for the given island (adapted from Neall and Trewick 2008). Distances g_{ij} report the shortest geographical distance from the coast of the row's area to the column's area (measured at present).

The paleogeographical information from Table 3 is encoded in three files named `hawaii.n4.times.txt`, `hawaii.n4.distances.txt`, and `hawaii.n4.connectivity.*.txt`.

```
geo_fn = "data/n4/hawaii.n4"
times_fn = geo_fn + ".times.txt"
dist_fn = geo_fn + ".distances.txt"
```

Create move index (`mvi`) and monitor index (`mni`) variables to populate the elements of our `moves` and `monitors` vectors, respectively.

```
mvi = 1
mni = 1
```

Read in the presence-absence range characters and record the number of areas in the dataset

```
dat_range_01 = readDiscreteCharacterData(range_fn)
n_areas <- dat_range_01.nchar()
```

Often, biogeographers wish to limit to the maximum allowable range size. This prohibits widespread species ranges and reduces the total number of range states in the analysis, thus improving computational efficiency. We will restrict ranges from including more than two areas. The total number of ranges equals $\sum_{k=0}^{m} \binom{n}{k}$ where n is the total number of areas, m is the maximum number of permissible areas, and $\binom{n}{k}$ is the number of ways to sample k unordered areas from a pool of n areas. For $n = 4$ and $m = 2$, this equals $\binom{4}{0} + \binom{4}{1} + \binom{4}{2} = 1 + 4 + 6 = 11$ states.

First, compute the number of states

```
max_areas <- 2
n_states <- 0
for (k in 0:max_areas) n_states += choose(n_areas, k)
```

then use `n_states` to format the dataset for the reduced state space

```
dat_range_n = formatDiscreteCharacterData(dat_range_01, "DEC", n_states)
```

Our state space now includes only 11 states (∅, K, O, M, H, KO, KM, OM, KH, OH, MH).

Record the complete list of range descriptions to file

```
state_desc = dat_range_n.getStateDescriptions()
state_desc_str = "state,range\n"
for (i in 1:state_desc.size())
{
    state_desc_str += (i-1) + "," + state_desc[i] + "\n"
}
write(state_desc_str, file=out_fn+".state_labels.txt")
```

As with the previous analysis, we'll brazenly assume we know the dated species phylogeny without error.

```
tree <- readTrees(tree_fn)[1]
```

Next, we'll read and structure our paleogeographic data. Read in the list of minimum and maximum ages of island formation

```
time_bounds <- readDataDelimitedFile(file=times_fn, delimiter=" ")
n_epochs <- time_bounds.size()
```

Read in the vector of matrices that describe the connectivity between areas over time. Note, there is one connectivity matrix per epoch, ordered from oldest to youngest.

```
for (i in 1:n_epochs) {
  epoch_fn[i] = geo_fn + ".connectivity." + i + ".txt"
  connectivity[i] <- readDataDelimitedFile(file=epoch_fn[i], delimiter=" ")
}
```

The area connectivity file for the third epoch (when K, O, and M exist, but not H) contains

```
1 1 1 0
1 1 1 0
1 1 1 0
0 0 0 0
```

Dispersal events between, say, K and M will be penalized by distance rather than be forbidden by non-connectivity.

Read in the matrix of distances between all pairs of areas (km). For simplicity, we will assume that distances remained constant across epochs, even though these distances certainly varied over time.

```
distances <- readDataDelimitedFile(file=dist_fn, delimiter=" ")
```

The distances files contains

```
001 145 239 419
145 001 059 239
239 059 001 082
419 239 082 001
```

and, if we assume the relative distance between islands remains roughly constant over time, then one set of distances is suitable for use for all four epochs.

Next, we'll build an enhanced DEC model. Like before, we'll define the rate matrix in terms of relative rates, then rescale the entire matrix with the biogeographic rate scaling parameter `rate_bg`.

```
log10_rate_bg ~ dnUniform(-4,2)
log10_rate_bg.setValue(-2)
rate_bg := 10^log10_rate_bg
moves[mvi++] = mvSlide(log10_rate_bg, weight=4)
```

Fix the base dispersal rate to 1

```
dispersal_rate <- 1.0
```

Dispersal rates might make use of some extrinsic information, such as geographical distances between areas (MacArthur and Wilson 1967; Webb and Ree 2012). We model this as $d_{ij} = \exp(-a g_{ij})$ where g_{ij} is the geographical distance between areas i and j and a is a parameter that scales distance. Note that all dispersal rates are equal when $a = 0$.

Add a distance scale parameter

```
distance_scale ~ dnUnif(0,20)
distance_scale.setValue(0.01)
moves[mvi++] = mvScale(distance_scale, weight=3)
```

Now we can assign rates that are functions of distance between all pairs of areas, *but also over all epochs*. To accomplish this, notice we now have an outer loop over the number of epochs, `n_epochs`. This is used to construct a vector of dispersal matrices, one matrix per epoch. It is crucial to note that all of elements are assigned the value `0.0` unless the if-statement `"if (connectivity[i][j][k] > 0)"` evaluates to `true`. That is, dispersal rates between areas `j` and `k` for epoch `i` are non-zero if and only if the connectivity matrix element `connectivity[i][j][k]` has a positive value! When this condition is met, the dispersal rate is determined by the exponential function of inverse distance given above.

```
for (i in 1:n_epochs) {
  for (j in 1:n_areas) {
    for (k in 1:n_areas) {
      dr[i][j][k] <- 0.0
      if (connectivity[i][j][k] > 0) {
        dr[i][j][k] := dispersal_rate * exp(-distance_scale * distances[j][k])
      }
    }
  }
}
```

We will assign the same extirpation prior as was done in the simple analysis in the previous section

```
log_sd <- 0.5
log_mean <- ln(1) - 0.5*log_sd^2
extirpation_rate ~ dnLognormal(mean=log_mean, sd=log_sd)
moves[mvi++] = mvScale(extirpation_rate, weight=2)
```

and then provide the appropriate extirpation matrix structure

```
for (i in 1:n_epochs) {
  for (j in 1:n_areas) {
    for (k in 1:n_areas) {
      er[i][j][k] <- 0.0
    }
    er[i][j][j] := extirpation_rate
  }
}
```

Now we have a vector of dispersal rates, `dr`, and an vector of extirpation rates, `er`, in stored in the `RevBayes` workspace. We'll use these to create a vector of four DEC rate matrices, one for each epoch.

```
for (i in 1:n_epochs) {
  Q_DEC[i] := fnDECRateMatrix(dispersalRates=dr[i],
                           extirpationRates=er[i],
                           maxRangeSize=max_areas)
}
```

Next, we need to define breakpoints for when the underlying paleogeographic state/connectivity changes. In our case, we'll define the epoch breakpoints as uniformly distributed random variables that are bounded by the minimum and maximum age estimates for when each new island complex formed (Table 3). This is easily done using a for loop over the number of epochs. Note, we define the end of the final epoch as the present.

```
for (i in 1:n_epochs) {
  time_max[i] <- time_bounds[i][1]
  time_min[i] <- time_bounds[i][2]
  if (i != n_epochs) {
      epoch_times[i] ~ dnUniform(time_min[i], time_max[i])
      moves[mvi++] = mvSlide(epoch_times[i], delta=(time_max[i]-time_min[i])/2)
  } else {
      epoch_times[i] <- 0.0
  }
}
```

Now that we have variables for the timing (`epoch_times`) and character (`Q_DEC` via `connectivity`) of paleogeographic change throughout the Hawaiian archipelago, we're ready to unify these objects with the `fnEpoch` function. This function requires a vector of rate matrices, a vector of epoch end times, and a vector of rate multipliers as arguments. Internally, the function computes the appropriate probabilities for state transitions along branches according under a piecewise constant continuous-time Markov chain. The important consequence of using an epoch model is that transition probabilities for anagenetic events depend on the geological age of the branch.

```
Q_DEC_epoch := fnEpoch(Q=Q_DEC, times=epoch_times, rates=rep(1,n_epochs))
```

Here, we treat the probability of different types of cladogenetic events as a random variables to be estimated.

```
clado_event_types <- [ "s", "a" ]
p_sympatry ~ dnUniform(0,1)
p_allopatry := abs(1.0 - p_sympatry)
clado_type_probs := simplex(p_sympatry, p_allopatry)
moves[mvi++] = mvSlide(p_sympatry, weight=2)
P_DEC := fnDECCladoProbs(eventProbs=clado_type_probs,
                       eventTypes=clado_event_types,
                       numCharacters=n_areas,
                       maxRangeSize=max_areas)
```

For this dataset, we assume cladogenetic probabilities are constant with respect to geological time. Using time-dependent cladogenetic probabilities (`fnEpochCladoProbs`) and mixtures of cladogenetic probabilities (`fnMixtureCladoProbs`) will be covered in future tutorials.

Among the four areas, only Kauai existed at the provided origination time of the clade, so will set it as the only valid starting state through the root frequency distribution.

```
rf_DEC <- rep(0, n_states)
rf_DEC[2] <- 1
rf_DEC <- simplex(rf_DEC)
```

We have created all the necessary model variables. Now we can create the phylogenetic model of anagenetic and cladogenetic character evolution. `dnPhyloCTMCClado` will internally make use of the time-heterogeneous probabilities embedded in the epoch rate generator, `Q_DEC_epoch`.

```
m_bg ~ dnPhyloCTMCClado(tree=tree,
                      Q=Q_DEC_epoch,
                      cladoProbs=P_DEC,
                      branchRates=rate_bg,
                      rootFrequencies=rf_DEC,
                      type="NaturalNumbers",
                      nSites=1)
```

Attach the observed range data to the distribution

```
m_bg.clamp(dat_range_n)
```

And the rest we've done before...

```
monitors[mni++] = mnScreen(printgen=100, rate_bg, extirpation_rate, distance_scale)
monitors[mni++] = mnModel(file=out_fn+".model.log", printgen=10)
monitors[mni++] = mnFile(tree, filename=out_fn+".tre", printgen=10)
monitors[mni++] = mnJointConditionalAncestralState(tree=tree,
                                                  ctmc=m_bg,
                                                  type="NaturalNumbers",
                                                  withTips=true,
                                                  withStartStates=true,
                                                  filename=out_fn+".states.log",
                                                  printgen=10)
```

Wrap the model graph into a model object

```
mymodel = model(m_bg)
```

then build and run MCMC

```
mymcmc = mcmc(mymodel, moves, monitors)
mymcmc.run(5000)
```

3.2 Results

Example results are located at `output_example/epoch.*`

When compared to the ancestral state estimates from the "simple" analysis (Figure 4), these results are far more consonant with what we understand about the origination times of the islands (Table 3). First, this reconstruction asserts that the clade originated in the modern Hawaiian islands at a time when only Kauai was above sea level. Similarly, the *D. sheriffiana* and *D. arborea* clade no longer estimates OMH as its ancestral range, since Maui and Hawaii had not yet formed 2.4 Ma. The ancestral range for the *Agyroxiphium* clade is Maui (M) with probability 0.41 and Maui+Hawaii (MH) with probability 0.33, whereas previously it gave high support to the range KMH.

It may be that these are relatively accurate historical biogeographic estimates, or they may contain artifacts as a result of assuming a fixed and errorless phylogeny. The next tutorials discuss how to jointly estimate phylogeny and biogeography, which potentially improves the estimation of divergence times, tree topology, and ancestral ranges.

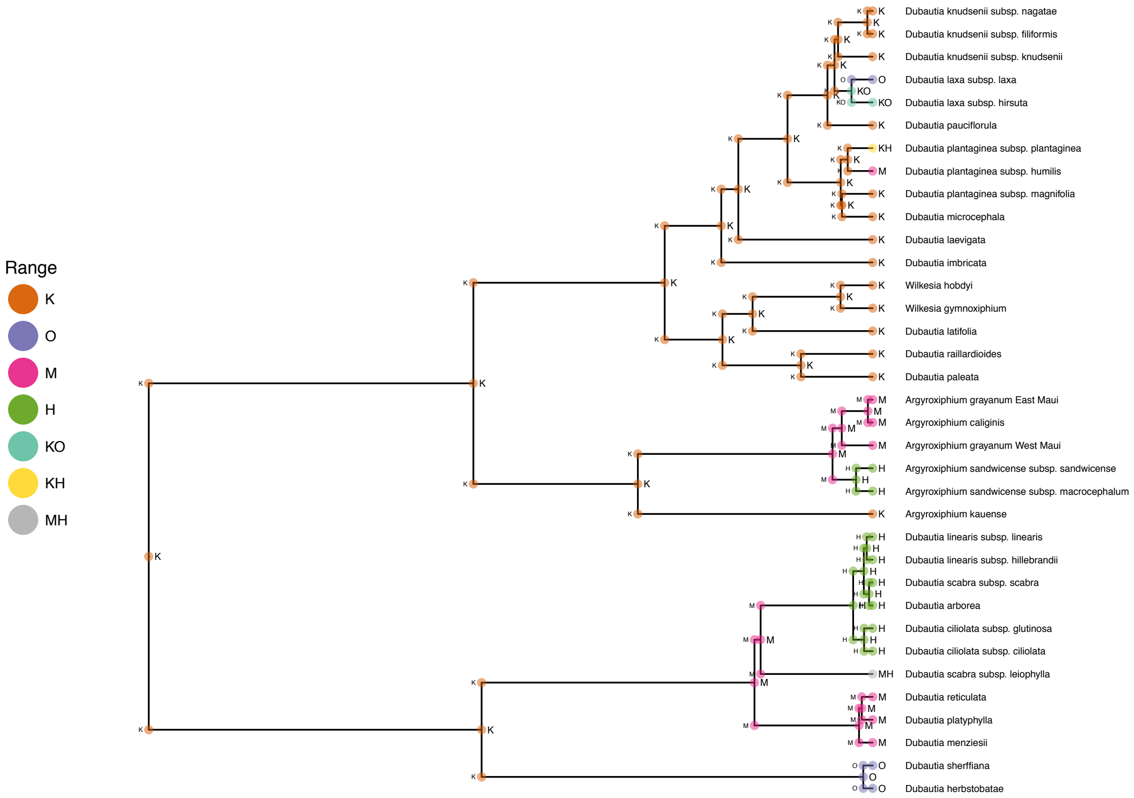

Range
K
O
M
H
KO
KH
MH
Dubautia knudsenii subsp. nagatae
Dubautia knudsenii subsp. filiformis
Dubautia knudsenii subsp. knudsenii
Dubautia laxa subsp. laxa
Dubautia laxa subsp. hirsuta
Dubautia pauciflorula
Dubautia plantaginea subsp. plantaginea
Dubautia plantaginea subsp. humilis
Dubautia plantaginea subsp. magnifolia
Dubautia microcephala
Dubautia laevigata
Dubautia imbricata
Wilkesia hobdyi
Wilkesia gymnoxiphium
Dubautia latifolia
Dubautia raillardioides
Dubautia paleata
Argyroxiphium grayanum East Maui
Argyroxiphium caliginis
Argyroxiphium grayanum West Maui
Argyroxiphium sandwicense subsp. sandwicense
Argyroxiphium sandwicense subsp. macrocephalum
Argyroxiphium kauense
Dubautia linearis subsp. linearis
Dubautia linearis subsp. hillebrandii
Dubautia scabra subsp. scabra
Dubautia arborea
Dubautia ciliolata subsp. glutinosa
Dubautia ciliolata subsp. ciliolata
Dubautia scabra subsp. leiophylla
Dubautia reticulata
Dubautia platyphylla
Dubautia menziesii
Dubautia sherffiana
Dubautia herbstobatae

Figure 5: Tree with ancestral state estimates. Nodes are annotated with ancestral states before and after cladogenetic events. Most probable states are shown. Colors of markers indicate the range state. Sizes of markers indicate the posterior probability of that state.

4 Biogeographic dating using DEC

This analysis will jointly estimate phylogeny and biogeography. One benefit is that the biogeographic analysis will intrinsically accommodate phylogenetic uncertainty, both in terms of topology and branch lengths. Another is that paleogeographic evidence has the potential provide information about the geological timing of speciation events in the phylogeny (Ho et al. 2015). Finally, biogeographic data may lend support to certain phylogenetic relationships that have poor resolution otherwise.

As mentioned in Section 2, Hawaiian silverswords are nested within the subtribe *Madiinae*, alongside the tarweeds, a clade of plants inhabiting in western North America. Fossil pollen evidence indicates that *Madiinae* diversified during a period of aridification from 15–5 Ma in the western regions of North America (Baldwin et al. 1991). It's clear that silverswords colonized Hawaii from western North America, but the timing of the event is difficult to estimate. Even though the oldest Hawaiian island they inhabit is Kauai, it is possible that silverswords first colonized older islands in the Emperor Island chain that predate the formation of Kauai (ca 5.1 Ma).

This makes the application of standard node-based biogeographic calibrations challenging, because it would require a strong assumption about when and how many times the oldest silversword lineages colonized Kauai. Did silverswords colonize Kauai once directly from the California coast? Or did the colonize the younger islands multiple times from older islands in the chain? And did the event occur immediately after Kauai surfaced or much later? Because we cannot observe the timing and nature of this event directly, we will integrate over all possible evolutionary histories using process-based biogeographic dating method described in Landis (2016).

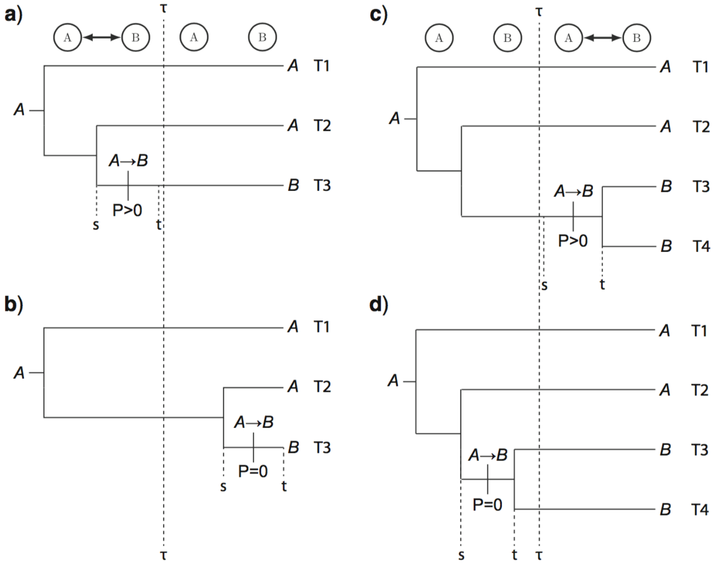


Figure 6: Cartoon of biogeographic transition probabilities as functions of geological time, and how that relates to speciation times. (a) Areas split, dispersal before split, positive probability; (b) Areas split, dispersal after split, zero probability; (c) Areas merge, dispersal after merge, positive probability; (d) Areas merge, dispersal before merge, zero probabilty. Original figure and details regarding cartoon assumptions are found in Landis (2016).

The basic idea is that an empirically informed epoch model is capable of creating conditions that favor key evolutionary transitions to occur during one time interval over another. Unlike the time-homogeneous probabilities that arise from, say, a molecular substitution process, these age-dependent transition probabilities may identify rate from time, and thus generate information about branch lengths in units of absolute time (Figure 6). A biogeographic process that is constrained by paleogeographic connectivity is well-suited to this purpose.

Note: like all dating methods, including node calibration methods, tip dating methods, and fossilized birth death dating methods, process-based biogeographic dating estimates are prior sensitive and dataset dependent. Applying this model to alternative data sets should be done with care!

Much of this tutorial will be similar to the previous sections, except we are adding a birth-death process and a molecular substitution process to the model graph.

4.1 Analysis

To use date the silversword radiation using biogeography, it is necessary that we transition from our simpler 4-area model to a richer 6-area model (see Figure 2). The mainland area (Z) is necessary to force the silversword and tarweed clade to originate apart from the islands. The area corresponding to the older island chain (R) is necessary because we do not know *a priori* whether silverswords colonized the modern islands directly from the mainland (Z → K), or first colonized R and only later dispersed into the younger islands any number of times (Z → R → K). Thus, adding these two areas allows the silversword origin time to precede the formation of Kauai when the dispersal rate is large.

Additionally, we will add three tarweed taxa to our dataset, increasing the total number of taxa to 38. We'll use a molecular alignment for the internal transcribed spacer (ITS) to estimate the phylogeny, which is a 657bp non-coding locus that is historically important for plant systematics. Because the locus is relatively short, it will also leave us with a fair amount of phylogenetic uncertainty in branch length and topology estimates. However, because we're estimating phylogeny and biogeography, it will be correctly incorporated into our ancestral range estimates.

As usual, we'll begin by creating variables to manage our input and output files

```
range_fn = "data/n6/silversword.n6.range.nex"
mol_fn = "data/n6/silversword.mol.nex"
tree_fn = "data/n6/silversword.tre"
out_fn = "output/test_epoch_phy"
geo_fn = "data/n6/hawaii.n6"
times_fn = geo_fn + ".times.txt"
dist_fn = geo_fn + ".distances.txt"
```

Add the analysis helper variables

```
mvi = 1
mni = 1
n_gen = 1e5   # more parameters, longer run!
```

Read in the molecular alignment

```
dat_mol = readDiscreteCharacterData(mol_fn)
```

Read in the species ranges for six areas

```
dat_range_01 = readDiscreteCharacterData(range_fn)
```

Compute the number of ranges when ranges may only be one or two areas in size

```
n_areas <- dat_range_01.nchar()
max_areas <- 2
n_states <- 0
for (k in 0:max_areas) n_states += choose(n_areas, k)
```

Then format the dataset for the reduced state space

```
dat_range_n = formatDiscreteCharacterData(dat_range_01, "DEC", n_states)
```

Record the complete list of range descriptions to file

```
state_desc = dat_range_n.getStateDescriptions()
state_desc_str = "state,range\n"
for (i in 1:state_desc.size())
{
    state_desc_str += (i-1) + "," + state_desc[i] + "\n"
}
write(state_desc_str, file=out_fn+".state_labels.txt")
```

Read the minimum and maximum ages of the island complexes

```
time_bounds <- readDataDelimitedFile(file=times_fn, delimiter=" ")
n_epochs <- time_bounds.size()
```

Read in the connectivity matrices between the six areas

```
for (i in 1:n_epochs) {
  epoch_fn[i] = geo_fn + ".connectivity." + i + ".txt"
  connectivity[i] <- readDataDelimitedFile(file=epoch_fn[i], delimiter=" ")
}
```

Read the geographical distances between areas

```
distances <- readDataDelimitedFile(file=dist_fn, delimiter=" ")
```

Remember that we are estimating the phylogeny as part of this analysis. In general, it is possible that certain combinations of phylogeny, biogeography, and paleogeography have zero-valued likelihoods should the epoch model introduce reducible rate matrix structures (see the supplemental of Buerki et al. 2011). The initial MCMC state, however, must have a non-zero probability for it to work properly. Although it may not be needed, we will provide `tree_init` as a starting tree for the `tree` variable that we will create to be safe.

```
tree_init = readTrees(tree_fn)[1]
```

We will record some basic information about the taxon set, the number of taxa, and the number of branches in the tree

```
taxa = tree_init.taxa()
n_taxa = taxa.size()
n_branches = 2 * n_taxa - 2
```

4.1.1 The tree model

Because we will estimate the topology and branch lengths parameters, the `tree` variable must be declared as a stochastic node with a prior distribution. For this, we'll use a constant rate birth-death process.

Assign root age with a maximum age of 15Ma to reflect the fossil pollen record for Californian tarweeds (Baldwin and Sanderson 1998). No assumption is made about the minimum root age.

```
root_age ~ dnUniform(0, 15)
moves[mvi++] = mvScale(root_age, weight=2)
```

Assign the proportion of sampled taxa (we have a non-uniform sampling scheme, but this should suffice).

```
rho <- 35/50
```

Assign the birth and death priors. It is important to note that the birth and death priors induce a root age distribution through the birth-death process. These priors generate a relatively uniform root age distribution between 2.5–15 Ma in the absence of data (i.e. running MCMC with the `underPrior=true` option).

```
birth ~ dnExp(1)
moves[mvi++] = mvScale(birth)
death ~ dnExp(1)
moves[mvi++] = mvScale(death)
```

Instantiate a tree variable generated by a birth-death process

```
tree ~ dnBDP(lambda=birth, mu=death, rho=rho, rootAge=root_age, taxa=taxa)
```

Add topology and branch length moves

```
moves[mvi++] = mvNNI(tree, weight=n_branches/2)
moves[mvi++] = mvFNPR(tree, weight=n_branches/8)
moves[mvi++] = mvNodeTimeSlideUniform(tree, weight=n_branches/2)
```

Provide a starting tree to ensure the biogeographic model has non-zero likelihood

```
tree.setValue(tree_init)
root_age.setValue(tree_init.rootAge())
```

4.1.2 The molecular model

To inform our branch lengths (in relative time units) and our topology, we will specify a simple HKY+Γ4+UCLN model of molecular substitution (Hasegawa et al. 1985; Yang and Nielsen 1998; Drummond et al. 2006).

First specify a base rate for the molecular clock. This prior is uniform over orders of magnitude, between 10^{-6} and 10^{3}, and was chosen to minimize its influence on the tree height.

```
log10_rate_mol ~ dnUniform(-6, 3)
log10_rate_mol.setValue(-1)
moves[mvi++] = mvSlide(log10_rate_mol, weight=5, delta=0.2)
rate_mol := 10^log10_rate_mol
```

Assign log-normal relaxed clock rate multipliers to each branch in the tree. These priors have a mean of 1 so each branch prefers a strict clock model in the absence of data.

```
branch_sd <- 1.0
branch_mean <- 0.0 - 0.5 * branch_sd^2
for (i in 1:n_branches) {
    branch_rate_multiplier[i] ~ dnLognormal(mean=branch_mean, sd=branch_sd)
    moves[mvi++] = mvScale(branch_rate_multiplier[i])
    branch_rates[i] := rate_mol * branch_rate_multiplier[i]
}
```

Now we'll create an HKY rate matrix. First, we create a Gamma-distributed transition-transversion (Ts/Tv) rate ratio with prior with mean equal to one

```
kappa ~ dnGamma(2,2)
moves[mvi++] = mvScale(kappa)
```

then create a flat Dirichlet prior on the base frequencies over A, C, G, and T

```
bf ~ dnDirichlet([1,1,1,1])
moves[mvi++] = mvSimplexElementScale(bf, alpha=10, weight=2)
```

and, finally, combine the base frequencies and Ts/Tv rate ratio to build the rate matrix

```
Q_mol := fnHKY(kappa, bf)
```

Next, we'll create a $+\Gamma4$ across-site rate variation model. First, we need a parameter to control the amount of site rate variation

```
alpha ~ dnUniform(0,50)
moves[mvi++] = mvScale(alpha)
```

and a discretized Gamma distribution with four categories

```
site_rates := fnDiscretizeGamma(alpha, alpha, 4)
```

The distribution of site rates categories has mean equal to one and variance equal to $1/\alpha$. When `alpha` grows small, the amount of site rate heterogeneity increases. When `alpha` is large, the variance shrinks to zero, and the site rate multipliers of `site_rates` converge to the value 1.

Finally, we'll create our molecular model of substitution

```
m_mol ~ dnPhyloCTMC(Q=Q_mol, tree=tree, branchRates=branch_rates, siteRates=site_rates,
   type="DNA", nSites=dat_mol.nchar())
```

and attach the ITS alignment

```
m_mol.clamp(dat_mol)
```

4.1.3 The biogeographic model

The biogeographic model is identical to that described in Section 3, so redundant details are omitted here.

First, create the biogeographic rate parameter.

```
log10_rate_bg ~ dnUniform(-4,2)
log10_rate_bg.setValue(-2)
rate_bg := 10^log10_rate_bg
moves[mvi++] = mvSlide(log10_rate_bg, weight=4)
```

The relative dispersal rate is fixed to 1

```
dispersal_rate <- 1.0
```

the distance scale parameter

```
distance_scale ~ dnUnif(0,20)
distance_scale.setValue(0.001)
moves[mvi++] = mvScale(distance_scale, weight=3)
```

Next, create dispersal rates that are functions of distance between all pairs of areas, but between areas that exist during epoch i!

```
for (i in 1:n_epochs) {
  for (j in 1:n_areas) {
    for (k in 1:n_areas) {
     dr[i][j][k] <- 0.0
     if (connectivity[i][j][k] > 0) {
       dr[i][j][k] := dispersal_rate * exp(-distance_scale * distances[j][k])
     }
    }
  }
}
```

Create the extirpation rates

```
log_sd <- 0.5
log_mean <- ln(1) - 0.5*log_sd^2
extirpation_rate ~ dnLognormal(mean=log_mean, sd=log_sd)
moves[mvi++] = mvScale(extirpation_rate, weight=2)

for (i in 1:n_epochs) {
  for (j in 1:n_areas) {
    for (k in 1:n_areas) {
      er[i][j][k] <- 0.0
    }
    er[i][j][j] := extirpation_rate
  }
}
```

Build a rate matrix for each time interval

```
for (i in 1:n_epochs) {
  Q_DEC[i] := fnDECRateMatrix(dispersalRates=dr[i],
                          extirpationRates=er[i],
                          maxRangeSize=max_areas)
}
```

Treat epoch times as random variables, except the present is always the present (or is it?).

```
for (i in 1:n_epochs) {
  time_max[i] <- time_bounds[i][1]
  time_min[i] <- time_bounds[i][2]
  if (i != n_epochs) {
    epoch_times[i] ~ dnUniform(time_min[i], time_max[i])
    moves[mvi++] = mvSlide(epoch_times[i], delta=(time_bounds[i][1]-time_bounds[i][2])
        /2)
  } else {
    epoch_times[i] <- 0.0
  }
}
```

Wrap the vector of rate matrices with the `fnEpoch` rate generator function

```
Q_DEC_epoch := fnEpoch(Q=Q_DEC, times=epoch_times, rates=rep(1, n_epochs))
```

Here, we treat the probability of different types of cladogenetic events as a random variable to be estimate.

```
clado_event_types <- [ "s", "a" ]
p_sympatry ~ dnUniform(0,1)
p_allopatry := abs(1.0 - p_sympatry)
moves[mvi++] = mvSlide(p_sympatry, delta=0.1, weight=2)
clado_event_probs := simplex(p_sympatry, p_allopatry)
P_DEC := fnDECCladoProbs(eventProbs=clado_event_probs,
                       eventTypes=clado_event_types,
                       numCharacters=n_areas,
                       maxRangeSize=max_areas)
```

Based on fossil pollen evidence, force range state and the root of the tree to be the mainland area (Z)

```
rf_DEC <- rep(0, n_states)
rf_DEC[n_areas+1] <- 1 # Mainland (Z) is the only possible starting state
rf_DEC <- simplex(rf_DEC)
```

Create the phylogenetic model of range evolution

```
m_bg ~ dnPhyloCTMCClado(tree=tree,
                        Q=Q_DEC_epoch,
                        cladoProbs=P_DEC,
                        branchRates=rate_bg,
                        rootFrequencies=rf_DEC,
                        type="NaturalNumbers",
                        nSites=1)
```

Attach the species range dataset to the model

```
m_bg.clamp(dat_range_n)
```

To easily identify interactions between the posterior estimates of island ages and divergence times, we'll create a deterministic node to monitor the age of the silversword radiation. First, create a deterministic node to monitor the crown age of the silversword radiation

```
ingroup_clade <- clade("Wilkesia_hobdyi",
                     "Dubautia_reticulata",
                     "Dubautia_microcephala",
                     "Argyroxiphium_caliginis")

ingroup_age := tmrca(tree, ingroup_clade)
```

Next, create a vector of variables to report the posterior probability that the clade originates *before* a given island. When the first argument in of the `ifelse` function returns `true`, the node has value `1` and `0` otherwise. Thus, the mean of this variable gives the posterior probability that the inequality is satisfied.

```
for (i in 1:n_epochs) {
  ingroup_older_island[i] := ifelse(ingroup_age > epoch_times[i], 1, 0)
}
```

Create the standard monitors. One difference is that the `mnFile` monitor will now record the posterior distribution for the `tree` variable, whereas the previous two tutorials assumed `tree` was fixed.

```
monitors[mni++] = mnScreen(printgen=100, ingroup_age)
monitors[mni++] = mnModel(file=out_fn+".model.log", printgen=100)
monitors[mni++] = mnFile(tree, filename=out_fn+".tre", printgen=100)
monitors[mni++] = mnJointConditionalAncestralState(tree=tree,
                                                  ctmc=m_bg,
                                                  type="NaturalNumbers",
                                                  withTips=true,
                                                  withStartStates=true,
                                                  filename=out_fn+".states.log",
                                                  printgen=100)
```

Because `ingroup_older_island` does not contribute to the model likelihood, it must be manually introduced to the model object. Compose the model object.

```
mymodel = model(m_bg, ingroup_older_island)
```

Create the MCMC object and run the analysis.

```
mymcmc = mcmc(mymodel, moves, monitors)
mymcmc.run(n_gen)
```

4.2 Results

Example results are located at `output_example/epoch_phy.* and output_example/simple_phy.*`

To understand the influence of the epoch model on ancestral range and divergence time estimation, it is important to run addition analyses with alternative settings. Scripts to jointly estimate molecular evolution, historical biogeographic, and phylogenetic parameters are available as `scripts/run_simple_phy.Rev` and `scripts/run_epoch_phy.Rev`. The "epoch" analysis is identical to the analysis just described. The "simple" analysis is similar to the "epoch" analysis, except it substitutes the paleogeography-aware model of range evolution (see Section 3) for a paleogeography-naive model (see Section 2).

We see that simple analysis (Figure 7) estimates the ancestral range at the root of the clade as Maui+Mainland (MZ). This is unrealistic, both because of the extreme distance between those areas, but also the simple

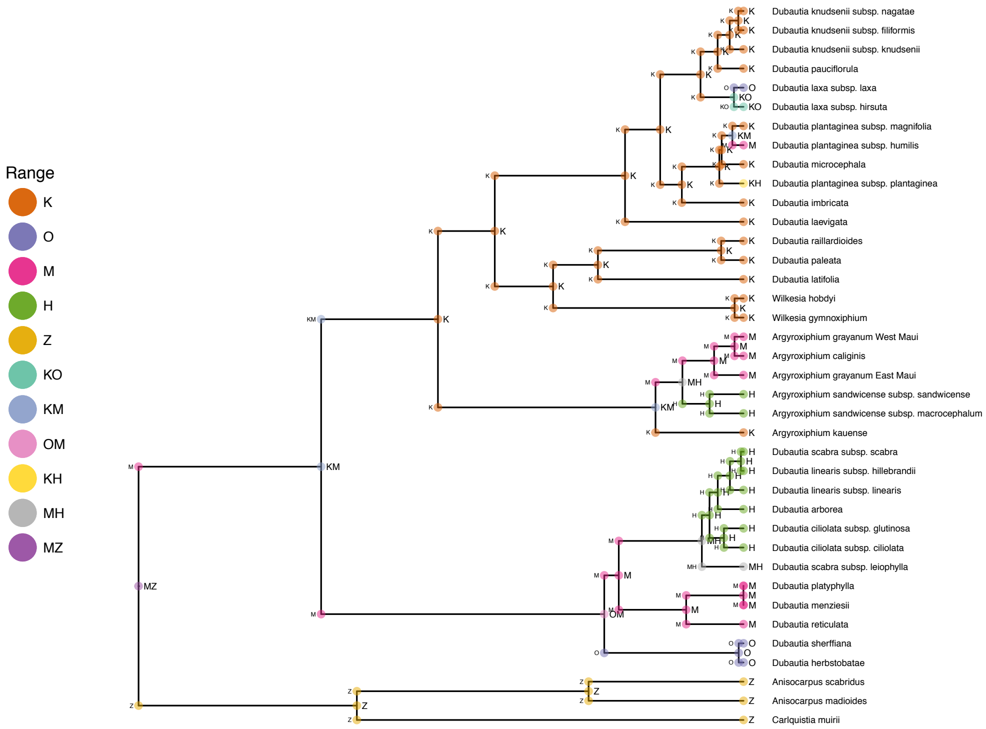

Range
K
O
M
H
Z
KO
KM
OM
KH
MH
MZ
K Dubautia knudsenii subsp. nagatae
K Dubautia knudsenii subsp. filiformis
K Dubautia knudsenii subsp. knudsenii
K Dubautia pauciflorula
O Dubautia laxa subsp. laxa
KO Dubautia laxa subsp. hirsuta
K Dubautia plantaginea subsp. magnifolia
M Dubautia plantaginea subsp. humilis
K Dubautia microcephala
KH Dubautia plantaginea subsp. plantaginea
K Dubautia imbricata
K Dubautia laevigata
K Dubautia raillardioides
K Dubautia paleata
K Dubautia latifolia
K Wilkesia hobdyi
K Wilkesia gymnoxiphium
M Argyroxiphium grayanum West Maui
M Argyroxiphium caliginis
M Argyroxiphium grayanum East Maui
H Argyroxiphium sandwicense subsp. sandwicense
H Argyroxiphium sandwicense subsp. macrocephalum
K Argyroxiphium kauense
H Dubautia scabra subsp. scabra
H Dubautia linearis subsp. hillebrandii
H Dubautia linearis subsp. linearis
H Dubautia arborea
H Dubautia ciliolata subsp. glutinosa
H Dubautia ciliolata subsp. ciliolata
MH Dubautia scabra subsp. leiophylla
M Dubautia platyphylla
M Dubautia menziesii
M Dubautia reticulata
O Dubautia sherffiana
O Dubautia herbstobatae
Z Anisocarpus scabridus
Z Anisocarpus madioides
Z Carlquistia muirii
KM
MZ
OM
MH

Figure 7: Joint estimate of phylogeny and biogeography, ignoring paleogeography.

analysis estimates the root age to be 10.3 (HPD95% 4.6, 15.0) Ma, well before Maui originated. (Date estimates are reported in the `simple_phy.mcc.tre` and `simple_phy.model.log` files.) The simple model also infers Kauai+Maui (KM) as the ancestral range of living silverswords and a crown age of 7.2 (HPD95% 2.5, 13.5) Ma, which is impossibly ancient given the islands' ages.

The epoch analysis (Figure 8) produces more sensible ancestral range estimates, with Kauai being colonized first, and younger islands only being colonized as they become available. The crown age of silverswords is estimated as 2.5 (HPD95% 0.7, 4.3) Ma. When comparing the results to the earlier fixed-phylogeny epoch results in Figure 5, we recover a greater role for cladogenesis for the younger speciation events. These two analyses only differ in terms of whether the phylogeny is fixed or estimated, so it is likely a result of phylogenetic error in the fixed tree.

In Tracer, one can look at the sampled posterior of island ages in comparison the origination time of crown silverswords (Figure 9). The left panel shows the simple analysis, where crown silverswords often originate before the formation of Kauai. The right panel shows that crown silverswords probably originated before the formation of Maui, but after the formation of Kauai.

By tabulating the results of the deterministic variable `ingroup_older_island`, we measure the posterior probability that crown silverswords originated before or after each particular epoch in the model (Table 4). Treating $P = 0.95$ as significant support for an evolutionary outcome, the epoch model produces strong support that crown silverswords originated after the formation of Kauai, $P(a_s > a_K) = 0.02 < 1 - 0.95$ and weak support that they originated after the formation of Oahu, $P(a_s > a_O) = 0.26 > 1 - 0.95$.

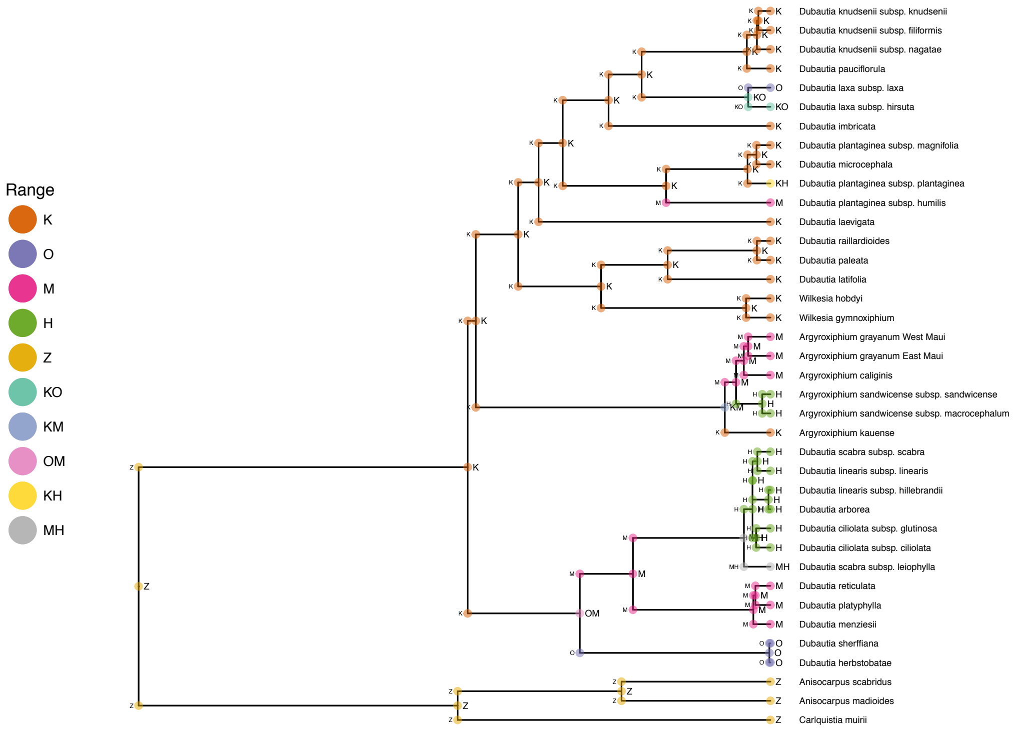

Range
K
O
M
H
Z
KO
KM
OM
KH
MH
Dubautia knudsenii subsp. knudsenii
Dubautia knudsenii subsp. filiformis
Dubautia knudsenii subsp. nagatae
Dubautia pauciflorula
Dubautia laxa subsp. laxa
Dubautia laxa subsp. hirsuta
Dubautia imbricata
Dubautia plantaginea subsp. magnifolia
Dubautia microcephala
Dubautia plantaginea subsp. plantaginea
Dubautia plantaginea subsp. humilis
Dubautia laevigata
Dubautia raillardioides
Dubautia paleata
Dubautia latifolia
Wilkesia hobdyi
Wilkesia gymnoxiphium
Argyroxiphium grayanum West Maui
Argyroxiphium grayanum East Maui
Argyroxiphium caliginis
Argyroxiphium sandwicense subsp. sandwicense
Argyroxiphium sandwicense subsp. macrocephalum
Argyroxiphium kauense
Dubautia scabra subsp. scabra
Dubautia linearis subsp. linearis
Dubautia linearis subsp. hillebrandii
Dubautia arborea
Dubautia ciliolata subsp. glutinosa
Dubautia ciliolata subsp. ciliolata
Dubautia scabra subsp. leiophylla
Dubautia reticulata
Dubautia platyphylla
Dubautia menziesii
Dubautia sherffiana
Dubautia herbstobatae
Anisocarpus scabridus
Anisocarpus madioides
Carlquistia muirii
Z
K
OM
KM

Figure 8: Joint estimate of phylogeny and biogeography, conditioning on paleogeography through the epoch model.

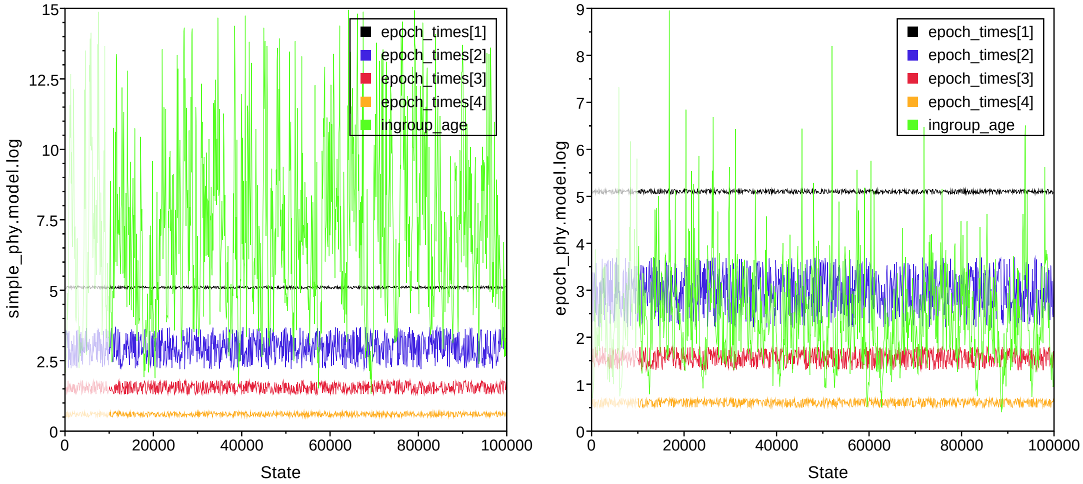


Figure 9: Plot of posterior samples for island ages and the origin time of living silverswords. The colors black, blue, red, orange, and green correspond to the origination times of Kaui, Oahu, Maui, Hawaii, and the silversword clade, respectively. The left panel ignores paleogeography, allowing silverswords to originate well before the formation of Kauai (`epoch_times[1]`). The right panel conditions of paleogeography, which prefers a silversword crown age that follows the formation of Kauai.

Model	$P(a_s > a_K)$	$P(a_s > a_O)$	$P(a_s > a_M)$	$P(a_s > a_H)$
simple	0.72	0.94	0.99	1.00
epoch	0.02	0.26	0.84	0.99

Table 4: Posterior probability that the age of crown silverswords (a_s) is older than the origination times of K, O, M, and H (a_K, a_O, a_M, a_H, respectively). The “simple” model (Left) ignores paleogeography while the “epoch” model (Right) conditions on it.

References

Baldwin, B. G., D. W. Kyhos, J. Dvorak, and G. D. Carr. 1991. Chloroplast DNA evidence for a North American origin of the Hawaiian silversword alliance (Asteraceae). Proceedings of the National Academy of Sciences 88:1840–1843.

Baldwin, B. G. and M. J. Sanderson. 1998. Age and rate of diversification of the Hawaiian silversword alliance (Compositae). Proceedings of the National Academy of Sciences 95:9402–9406.

Buerki, S., F. Forest, N. Alvarez, J. A. Nylander, N. Arrigo, and I. Sanmartín. 2011. An evaluation of new parsimony-based versus parametric inference methods in biogeography: a case study using the globally distributed plant family Sapindaceae. Journal of Biogeography 38:531–550.

Carlquist, S. 1959. Studies on Madinae: anatomy, cytology, and evolutionary relationships. Aliso 4:171–236.

Drummond, A., S. Ho, M. Phillips, and A. Rambaut. 2006. Relaxed Phylogenetics and Dating with Confidence. PLoS Biology 4:e88.

Gillespie, G. R. and G. B. Baldwin. 2009. Island Biogeography of Remote Archipelagoes. The Theory of Island Biogeography Revisited Pages 358–387.

Hasegawa, M., H. Kishino, and T. Yano. 1985. Dating of the human-ape splitting by a molecular clock of mitochondrial DNA. Journal of Molecular Evolution 22:160–174.

Ho, S. Y., K. J. Tong, C. S. Foster, A. M. Ritchie, N. Lo, and M. D. Crisp. 2015. Biogeographic calibrations for the molecular clock. Biology Letters 11:20150194.

Landis, M. J. 2016. Biogeographic dating of speciation times using paleogeographically informed processes. Systematic Biology Advance Access.

Landis, M. J., N. J. Matzke, B. R. Moore, and J. P. Huelsenbeck. 2013. Bayesian analysis of biogeography when the number of areas is large. Systematic Biology 62:789–804.

MacArthur, R. H. and E. O. Wilson. 1967. Theory of Island Biogeography. vol. 1. Princeton University Press.

Massana, K. A., J. M. Beaulieu, N. J. Matzke, and B. C. O’Meara. 2015. Non-null effects of the null range in biogeographic models: Exploring parameter estimation in the dec model. bioRxiv Page 026914.

Matzke, N. J. 2012. Founder-event speciation in BioGeoBEARS package dramatically improves likelihoods and alters parameter inference in dispersal–extinction–cladogenesis DEC analyses. Frontiers of Biogeography 4:210.

Neall, V. E. and S. A. Trewick. 2008. The age and origin of the Pacific islands: a geological overview. Philosophical Transactions of the Royal Society B: Biological Sciences 363:3293–3308.

Ree, R. H., B. R. Moore, C. O. Webb, M. J. Donoghue, and K. Crandall. 2005. A likelihood framework for inferring the evolution of geographic range on phylogenetic trees. Evolution 59:2299–2311.

Ree, R. H. and S. A. Smith. 2008. Maximum likelihood inference of geographic range evolution by dispersal, local extinction, and cladogenesis. Systematic Biology 57:4–14.

Webb, C. O. and R. Ree. 2012. Historical biogeography inference in malesia. Biotic evolution and environmental change in Southeast Asia Pages 191–215.

Yang, Z. and R. Nielsen. 1998. Synonymous and nonsynonymous rate variation in nuclear genes of mammals. Journal of Molecular Evolution 46:409–418.

Version dated: March 13, 2017